

ENERGY DEGRADATION OF ELECTRONS
IN ATMOSPHERIC GASES

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TABLE OF CONTENTS

	Page
ACKNOWLEDGEMENTS	ii
LIST OF TABLES	vi
LIST OF FIGURES.	viii
Chapter	
I. INTRODUCTION.	1
II. CROSS SECTION RULES	3
1. <u>Introduction</u>	3
2. <u>The Born Approximation and Generalized</u> <u>Oscillator Strengths</u>	3
3. <u>Allowed Transitions</u>	9
4. <u>Forbidden Transitions</u>	13
5. <u>Rydberg Series</u>	14
6. <u>Ionizing Transitions</u>	17
7. <u>Application to Atomic Oxygen</u>	19
III. MOLECULAR NITROGEN.	28
1. <u>Introduction</u>	28
2. <u>Analytic Excitation Cross Sections</u>	29
3. <u>Allowed Transitions</u>	33
4. <u>Forbidden Transitions</u>	49
5. <u>Ionization Continuum</u>	49
6. <u>Franck-Condon Factors and Vibrational Excitation</u> . .	60

Chapter	Page
IV. MOLECULAR OXYGEN.	63
1. <u>Introduction</u>	63
2. <u>Allowed Transitions</u>	63
3. <u>Forbidden Transitions</u>	76
4. <u>Ionization Continuum</u>	76
5. <u>Vibrational Excitation</u>	85
V. ENERGY LOSS	86
1. <u>Energy Loss per cm. Path (Stopping Power)</u>	86
2. <u>Excitation Loss - Electronic States</u>	88
3. <u>Ionization Loss</u>	90
4. <u>Energy Loss of Very Slow Electrons</u>	91
VI. SECONDARY ELECTRONS	93
1. <u>Secondary Spectrum</u>	93
2. <u>Degradation of Secondary Spectrum</u>	95
3. <u>Tertiary Spectrum and Its Degradation</u>	96
4. <u>Summary of Complete Energy Degradation</u>	97
VII. DEGRADATION IN GASEOUS MIXTURES	99
1. <u>Energy Transfer Functions</u>	99
2. <u>Secondary Distributions</u>	102
3. <u>Examples of Excited State Population Calculations</u> .	107
a. Photoelectrons.	107
b. Auroral Electrons	111
4. <u>Radiation from Excited States</u>	150
5. <u>Corrections for Quenching</u>	154
6. <u>Discussion of Results</u>	156

	Page
REFERENCES	159
BIOGRAPHICAL SKETCH.	163

LIST OF TABLES

Table	Page
1. Atomic Oxygen Parameters.	24
2. Ionization Parameters for Atomic Oxygen	27
3. N ₂ Allowed Parameters	36
4. Rydberg Series Levels and Oscillator Strengths.	38
5. Relative Sizes of Ionization Continua	44
6. N ₂ Parameters for Forbidden States.	54
7. N ₂ Ionization Parameters.	57
8. O ₂ Allowed Parameters	69
9. O ₂ Rydberg Series	70
10. O ₂ Relative Sizes of Ionization Continua.	71
11. O ₂ Forbidden Parameters	79
12. O ₂ Ionization Parameters.	82
13. Photoelectron Groups.	110
14. Photoelectron Degradation	112
15. Energy Deposition of a 30 keV Electron.	116
16. Energy Deposition of a 10 keV Electron.	124
17. Energy Deposition of a 1 keV Electron	132
18. Energy Deposition of a 0.1 keV Electron	140
19. Energy into Species	148
20. Energy into Ions and eV per Ion Pair.	149
21. Airglow Features.	151

Table	Page
22. Auroral Features.	155
23. Quenching Coefficients and Corrections.	157

LIST OF FIGURES

Figure	Page
1. Relationship between the momentum transfer and the incoming and outgoing momenta	8
2. Allowed cross section forms	12
3. Forbidden cross section forms	16
4. Ionization cross section forms.	21
5. Energy levels of atomic oxygen.	23
6. Energy levels of N_2	35
7. Impact spectrum for a typical Rydberg series and ionization continuum.	41
8. Zero angle impact spectrum of N_2	43
9. Allowed generalized oscillator strengths for N_2	46
10. Allowed cross sections for N_2 -12.85 and 14.0 peaks.	48
11. Allowed cross sections - higher Rydberg series members	51
12. Forbidden cross sections.	53
13. Ionization cross sections	59
14. Energy levels of O_2	65
15. Zero angle impact spectrum of O_2	68
16. Allowed generalized oscillator strengths of O_2	73
17. Allowed cross sections - 8.4 and 9.9 eV peaks	75
18. Allowed cross sections - higher Rydberg series members	78

Figure	Page
19. Forbidden cross sections.	81
20. Ionization cross sections	84
21. E-E' integration plane.	94
22. Energy transfer curves for selected states in N_2 , O_2 and O.	101
23. Reciprocal loss function.	104
24. Secondary spectra	106
25. Tertiary spectra.	109

CHAPTER I

INTRODUCTION

The problem of the loss of energy of charged particles traversing matter has been studied many times before.¹⁻⁴ These studies have had in common the inability to cope with the low energy electrons formed in ionization. This inability was a direct result of the lack of information on low energy (below the Born approximation range) electron impact cross sections. This dissertation begins with a phenomenological analysis of cross sections for electron impact on atomic oxygen, molecular nitrogen and molecular oxygen in Chapters II, III and IV. Chapter II consists of the application to atomic oxygen of a set of phenomenological rules derived from studies of helium by Green and Dutta⁵ and Jusick, Watson and Green.⁶ The cross sections of this chapter will be sent to the Journal of Geophysical Research for publication by Dr. A. T. Jusick and Professor Green.⁷ Their analyses are based on a low energy extrapolation of the Born approximation. Chapters III and IV are phenomenological analyses of molecular nitrogen and oxygen cross sections relying heavily upon the experimental data of Lassettre, et al.,⁸⁻¹⁷ and the phenomenological methods of Green and Dutta and Jusick, Watson and Green. These two chapters, with only minor changes, will be sent to the Journal of Geophysical Research and represent the work of Drs. Charles Watson and Victor Dulock in addition to Professor Green and myself.

The next two chapters consider the equations dealing with the energy loss of charged particles traversing matter. The energy loss calculations require a knowledge of the cross sections for all important processes at all relevant energies. The discussion is phrased in terms of electrons but would work equally as well for heavier charged particles by substituting the corresponding cross sections. Throughout the calculations there is no consideration of the spatial or time scales of the processes, only that there is a sufficient quantity of the target gas to completely stop the incident particles. Hence, when we say an electron slowing down leaves a certain amount of energy in a particular excited state, we mean that this quantity has been integrated over the complete path of the incident electron and all of its secondaries.

Chapter VII considers the actual calculational procedures used along with a short discussion of some of the possible applications to atmospheric problems. In particular, the application of these energy degradation calculations to auroral electrons is discussed. This represents the second generation of a calculation on the degradation of 30 keV electrons by Green and Barth.¹⁸ In the present calculation, the detailed spectrum of the secondaries and tertiaries are considered and the cross sections used are from a more recent analysis.

It must be noted that these calculations are not an end in themselves as far as atmospheric applications are concerned but are meant as a tool to be used with a detailed atmospheric model to calculate observable radiation from a knowledge of the energy spectrum of input particles.

CHAPTER II

CROSS SECTION RULES

1. Introduction

In any study of particle energy loss it is necessary to know the cross sections for all relevant processes. For the case of electron-atom and electron-molecule scattering with which we are concerned, knowledge of the cross sections is the most difficult part of the problem. Few of the relevant cross sections have been measured or calculated over the entire energy range of interest. It would therefore be useful to formulate rules for obtaining complete sets of electron impact cross sections from the limited data and theory available. This chapter is devoted to the formulation of these rules in which we relate allowed transitions to optical oscillator strengths and forbidden transitions to allowed transitions. We also consider Rydberg series leading to the various continua and the ionization continua themselves, formulating rules to obtain cross sections from a limited amount of data. For molecules the relationship between the cross section to a particular vibrational state and the Franck-Condon factor is discussed along with the relationship of the previously mentioned rules for molecular cross sections.

2. The Born Approximation and Generalized Oscillator Strengths

The Born approximation provides a handy tool for obtaining high energy cross sections and as we shall see, leads to the concept of

the generalized oscillator strength which in turn, in the limit of zero momentum transfer, reduces to the optical oscillator strength. The optical oscillator strength is proportional to the probability of excitation by photon impact and is a fairly widely tabulated quantity. Because the optical oscillator strength is a limit of the generalized oscillator strength it serves as a means of normalizing allowed electron impact cross sections. The development of this section follows that of Mott and Massey.¹⁹

The differential cross section for inelastic electron impact is given by the well known formula

$$I_{mn}(K)dK = \frac{8\pi^2 m^2}{h^4} \frac{KdK}{k^2} \left| \iiint V e^{iKX} \psi_m \psi_n^* d\vec{r} d\vec{R} \right|^2 \quad (1)$$

where $K\hat{n}$ denotes the momentum transfer, $\vec{R}$ denotes the coordinates of the incident electron, $\vec{r}$ denotes the coordinates of the atomic electron, ψ_m is the wave function of the initial state, ψ_n is the wave function of the final state and V is the interaction potential. For the Coulomb potential the integral over the atomic electron coordinates can be evaluated

$$\int V e^{iKX} d\vec{R} = \epsilon^2 \sum_{s=1}^Z \int \frac{e^{iKX}}{|\vec{R}-\vec{r}_s|} d\vec{R} \quad (2)$$

where ϵ is the electronic charge and the index s runs over all Z atomic electrons. The evaluation is carried out by means of the formula

$$\int \frac{\exp(iK\hat{n} \cdot \vec{r}')}{|\vec{r}-\vec{r}'|} d\vec{r}' = \frac{4\pi}{K^2} e^{iK\hat{n} \cdot \vec{r}}. \quad (3)$$

Therefore

$$\int V e^{iKX} d\vec{R} = \frac{4\pi\epsilon^2}{K^2} \sum_{s=1}^Z e^{iKx_s}. \quad (4)$$

Thus the differential cross section is

$$I_{mn}(K) dK = \frac{128\pi^5 m^2 e^4}{k^2 h^4} \frac{dK}{K^3} |\epsilon_{mn}(K)|^2 \quad (5)$$

where

$$\epsilon_{mn}(K) = \sum_{s=1}^Z \int e^{iKx_s} \psi_m^* \psi_n^* d\vec{r}. \quad (6)$$

We can establish a relationship between $|\epsilon_{mn}(K)|^2$ and the dipole transition probability by expanding the e^{iKx} in the integral for the one electron case

$$e^{iKx} = 1 + iKx - \frac{K^2 x^2}{2!} - i \frac{K^3 x^3}{3!} + \dots \quad (7)$$

Thus

$$\epsilon_{mn}(K) = \int \psi_m \psi_n^* d\vec{r} + iK \int \psi_m x \psi_n^* d\vec{r} + \dots \quad (8)$$

where the first term is zero because of the orthogonality of ψ_m and ψ_n and the second term is the dipole matrix element. Therefore, to terms of the order of K^2

$$|\epsilon_{mn}(K)|^2 = K^2 \int \psi_m x \psi_n^* d\vec{r} + O(K^3). \quad (9)$$

The optical transition probability for a dipole transition is

$$\phi_{mn} = \frac{|X_{mn}|^2}{a_0^2} \quad (10)$$

where

$$X_{mn} = \int \psi_m x \psi_n^* d\vec{r} \quad (11)$$

and $a_0 = \hbar^2/m^2 e^4$ is the Bohr radius. Analogously the generalized

transition probability is defined as

$$\phi_{mn}(K) = \frac{|\epsilon_{mn}(K)|^2}{a_0^2 K^2} \quad (12)$$

where in the limit $K \rightarrow 0$ $|\epsilon_{mn}(K)|^2$ approaches $K^2 |X_{mn}|^2$ and $\phi_{mn}(K)$ is seen to approach ϕ_{mn} . We now define the concept of an oscillator strength which for optical transitions is

$$f_{mn} \equiv \frac{\nu_{mn}}{cR} \phi_{mn} \quad (13)$$

where $\nu_{mn} = (E_n - E_m)/h$ is the frequency associated with the transition and $R = 2\pi^2 me^4 / ch^3$ is the Rydberg constant. Analogously the generalized oscillator strength is defined as

$$f_{mn}(K) = (E_n - E_m) \frac{2m}{K^2 h^2} |\epsilon_{mn}(K)|^2 \quad (14)$$

and the differential cross section in terms of the generalized oscillator strength is

$$I_{mn}(K) dK = \frac{2\pi e^4}{EW} f_{mn}(K) \frac{dK}{K} \quad (15)$$

where $E = \frac{\hbar^2 k^2}{2m}$ is the incident energy and $W = E_n - E_m$ is the energy loss. The constant may be rewritten by noting that $e^4 = \left(\frac{e^2}{a_0}\right)^2 a_0^2 = (2R_e)^2 a_0^2$ where $R_e = 13.6$ eV is the Rydberg energy. Making a transformation to the variable $x = a_0^2 K^2$ we may rewrite the differential cross section as

$$I_{mn}(x) dx = \frac{\pi a_0^2 (2R_e)^2}{WE} f_{mn}(x) \frac{dx}{x}. \quad (16)$$

We then define $q_0 = \pi a_0^2 (2R_e)^2$ which is a universal constant which will multiply all cross sections. If the value of q_0 is calculated using

R_e in eV then the differential cross section is obtained by substituting E and W in eV. The value of q_0 is

$$q_0 = 6.513 \times 10^{-14} \text{ cm}^2 \text{ eV}^2. \quad (17)$$

The total cross section as a function of E is then obtained by integrating over x

$$\sigma_{mn}(E) = \int_{x_\ell}^{x_u} I_{mn}(x) dx = \frac{q_0}{EW} \int_{x_\ell}^{x_u} \frac{f_{mn}(x)}{x} dx \quad (18)$$

where the limits x_ℓ and x_u are obtained from the relationship

$$K^2 = k^2 + k_n^2 - 2kk_n \cos\theta. \quad (19)$$

This relationship is illustrated in Figure 1 where $\vec{k}$ is the incident wave vector, $\vec{k}_n$ is the scattered wave vector and $\vec{K}$ is the difference. This can be rewritten as

$$x = \frac{W}{R_e} \left(\frac{2E}{W} - 1 - 2\sqrt{\frac{E}{W} \left(\frac{E}{W} - 1 \right)} \cos\theta \right). \quad (20)$$

The limits x_ℓ and x_u are found from forward and backward scattering respectively. These limits are

$$x_\ell = \frac{W}{R_e} \left(\frac{2E}{W} - 1 - 2\sqrt{\frac{E}{W} \left(\frac{E}{W} - 1 \right)} \right) \quad (21)$$

and

$$x_u = \frac{W}{R_e} \left(\frac{2E}{W} - 1 + 2\sqrt{\frac{E}{W} \left(\frac{E}{W} - 1 \right)} \right). \quad (22)$$

From Eq.(18) we see that if the optical oscillator strength (we will now call it f_0) can be used as a magnitude setting parameter we may rewrite $f_{mn}(x)$ as $f_0 G_{mn}(x)$ where $G_{mn}(x)$ contains all of the x dependence

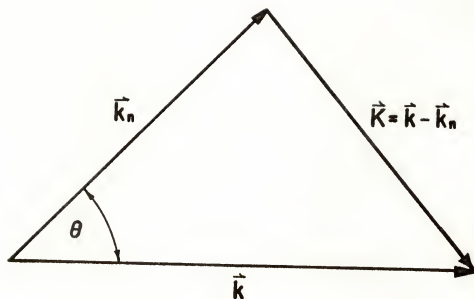


Fig. 1. Relationship between the momentum transfer and the incoming and outgoing momenta. $\vec{K}$ is the momentum transfer, $\vec{k}$ is the incoming momentum and $\vec{k}_n$ is the outgoing momentum.

and f_0 may be taken outside of the integral. Therefore Eq.(18) may be rewritten

$$\sigma_{mn}(E) = \frac{q_0 f_0}{W} \frac{W}{E} \int_{x_l}^{x_u} \frac{G_{mn}(x)}{x} dx = \frac{q_0 f_0}{W} g(\epsilon) \quad (23)$$

where $\epsilon = \frac{E}{W}$ and

$$g(\epsilon) = \frac{1}{\epsilon} \int_{x_l}^{x_u} \frac{G_{mn}(x)}{x} dx \quad (24)$$

is a function which contains all of the energy dependence of the cross section. In the next sections of the chapter we will discuss some phenomenological representations of the $g(\epsilon)$ functions both in the Born region and the lower energy region.

3. Allowed Transitions

Consider electron-excitation cross sections in which an atom or molecule is excited to a state at energy W by an electron which initially has the energy E . As shown in the previous section all of these excitation cross sections can in the Born approximation be placed in the form

$$\sigma(\epsilon) = \frac{q_0 f_0}{W^2} g(\epsilon). \quad (25)$$

It is then not unreasonable to assume that this type of form represents the cross section at all energies. Of course the energy dependence at low energies where the Born approximation is not valid will be changed somewhat but there still will exist some function $g(\epsilon)$ which will represent the cross section.

In the excitation of a state connected to the ground state via an allowed transition, cross sections have the characteristic of rising

from zero at the threshold according to some simple power law, reaching a maximum, leveling off, and ultimately falling off more or less in an $E^{-1} \log E$ fashion suggested by the Born approximation. This general type of behavior can be conveniently represented by the one-parameter function²¹

$$g(\epsilon, \alpha) = \left(1 - \frac{1}{\epsilon}\right) \frac{1}{\epsilon} \ln \frac{2.246\epsilon}{\alpha}. \quad (26)$$

In the absence of any other evidence concerning the choice of α , the choice $\alpha = 2$ yields a good fit to Seaton's²⁰ results and gives the function

$$g(\epsilon) = \left(1 - \frac{1}{\epsilon}\right) \frac{1}{\epsilon} \ln 1.123\epsilon. \quad (27)$$

Further analytic convenience can be achieved by replacing the logarithm by an appropriate power law. This gives the analytic form of Green and Barth¹⁸

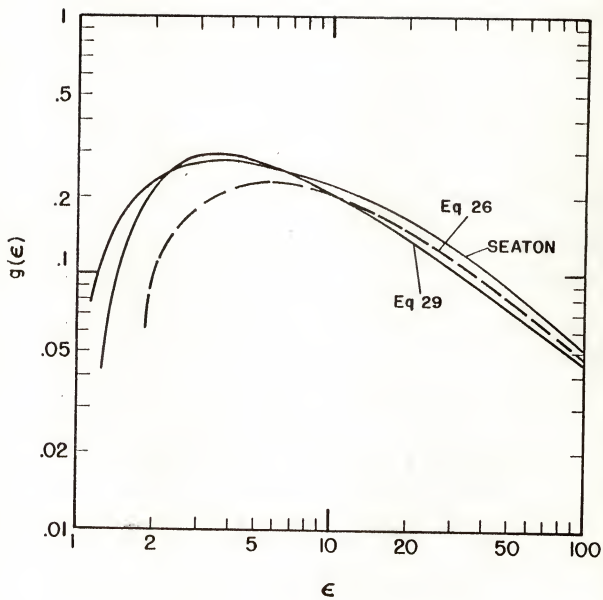
$$g(\epsilon) = C_0 \left(1 - \frac{1}{\epsilon}\right) \left(\frac{1}{\epsilon}\right)^{1-\omega} \quad (28)$$

where we can now choose the parameters to give a good fit to Seaton's results. A good choice is

$$g(\epsilon) = 1.5 \left(1 - \frac{1}{\epsilon}\right)^2 \left(\frac{1}{\epsilon}\right)^{0.75} \quad (29)$$

where the parameter $\omega = 2$ is chosen to be an integer because of analytic convenience obtained in doing some of the integrations involved in the energy degradation. Figure 2 shows Seaton's results along with Eqs.(26) and (29).

Figure 2. Allowed cross section forms.



In the case of allowed states the magnitude of the cross section is governed by the optical oscillator strength, which is essentially the square of the dipole matrix element. In the next section we will consider forbidden transitions in which the optical oscillator strength is zero and another parameter must be obtained to set the magnitude of the cross sections.

4. Forbidden Transitions

Forbidden transitions can be roughly divided into two groups, spin-flip and non-spin-flip. Non-spin-flip forbidden transitions are generally electric quadrupole transitions which violate the $|\Delta l| = 1$ dipole selection rule. A good representation of the cross section may be obtained with

$$\sigma(E) = \frac{q_0}{W^2} Q \left(1 - \frac{1}{\epsilon}\right) \frac{1}{\epsilon} \quad (30)$$

where the dependence upon ϵ was determined from approximate fits to the He cross sections of Jusick, Watson and Green.⁶ The magnitude parameter Q is related to the quadrupole matrix element and can be determined approximately by comparison with the corresponding $|\Delta l| = 1$ allowed optical oscillator strength. Thus we set $Q = a f_0$ and find $a \approx 0.1$ from the He cross sections of Jusick, Watson and Green.

For spin-flip transitions the exchange term usually plays a dominant role. These transitions are strictly forbidden under dipole selection rules and always exhibit very sharply peaked cross sections as a function of energy. Again, approximate fitting of the analytic form of Green and Barth to the He cross sections of Jusick, Watson and Green yields

$$\sigma(\epsilon) = \frac{q_0 f'_0}{W^2} \left(1 - \frac{1}{\epsilon}\right) \left(\frac{1}{\epsilon}\right)^2 \quad (31)$$

where $f'_0 = af_0$ and $a \approx 0.3$ except for the $1s \rightarrow 3D$, $\Delta s = 1$, $\Delta l = 2$ transition for which a better choice seemed to be $a \approx 0.1$. Figure 3 shows the $g(\epsilon)$ parts of Eqs.(30) and (31).

5. Rydberg Series

When an electron is excited to states of higher and higher principle quantum number n its orbit is soon outside of the orbits of the other electrons and it sees the potential of the nucleus minus that of the other electrons. Thus the electron is seeing an essentially hydrogenic potential and the energy levels and cross sections exhibit the characteristics of the Rydberg series of levels in hydrogen. That is, the energies follow the formula

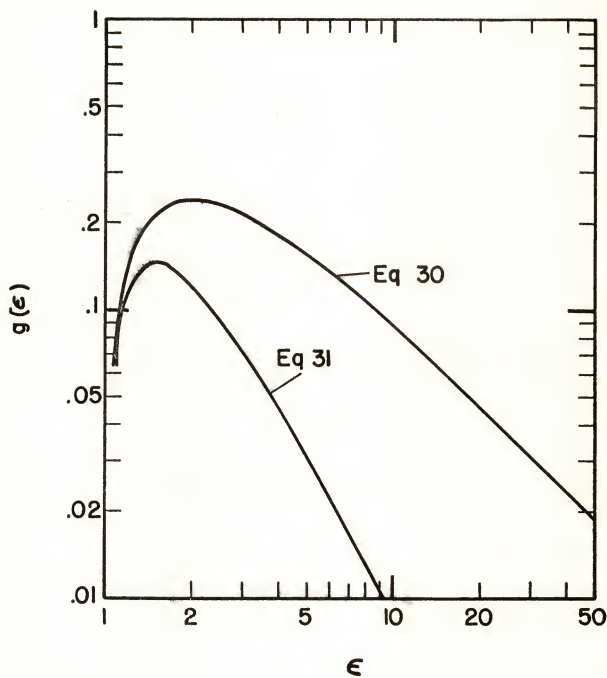
$$E_n = E_{\text{lim}} - R_e / n^{*2} = E_{\text{lim}} - R_e / (n - \sigma)^2. \quad (32)$$

E_{lim} is the energy of the series limit at which the outer electron becomes fully detached; $R_e = 13.6$ eV is the ionization energy of the H atom; n is the principle quantum number; $n^* = n - \sigma$ is the effective quantum number; and σ is the quantum defect. A convenient rule for the determination of the magnitude of the cross sections for the members of a Rydberg series is⁵

$$f_n = \frac{c}{n^{*3}} = \frac{c}{(n - \sigma)^3}. \quad (33)$$

We see that from the preceding sections we can phenomenologically represent the cross sections of all excitations through knowledge

Figure 3. Forbidden cross section forms.



of one optical oscillator strength for each allowed series. The optical oscillator strengths can then be found in the tabulations of Allen,²² Griem²³ and Kelly.²⁴

6. Ionizing Transitions

An ionization cross section may be viewed as a sum of excitation cross sections to the continuum of states above the ionization threshold. Accordingly, to apply the work on excitation cross sections we must in some way, be able to identify the effective cross section per interval of energy loss. In pursuing the phenomenological approach it is not unreasonable to accept the identical functional form for the differential energy loss cross section as for excitation to discrete states provided we regard W now as a continuous variable which ranges from the ionization threshold I to $E_m = (E+I)/2$. This upper limit should be used when experimental differential energy loss cross sections are used or when theoretical calculations are used which allow for the indistinguishability of the incident and secondary electron. Denoting this differential energy loss function by $S(E,W)$ we have for the ionization cross section

$$\sigma(E) = \int_I^{E_m} S(E,W) dW = q_o f_o \int_I^{E_m} \frac{C(W)}{W} \left(1 - \frac{W}{E}\right)^{\nu} \left(\frac{W}{E}\right)^{1-\omega} dW \quad (34)$$

where we here indicate that $C(W)$ may also vary with W . In the absence of detailed guidance of a purely theoretical nature, we explore the possible forms of $C(W)$ on the basis of data derived from the studies of Silverman and Lassette^{8,15} on molecular oxygen and nitrogen generalized oscillator strengths. In both cases we find that when $C(W)$ has an inverse power law dependence, that is

$$C(W) = C_0 \left(\frac{I}{W} \right)^p \quad (35)$$

with $p \approx 1.5$, Eq.(34) provides a reasonable representation of the W dependence of $S(E,W)$.

For many applications such as the calculation of energy loss and secondary electron distributions, it is not sufficient to know just the ionization cross section. Instead, the differential ionization cross section contains the required information. For example, to calculate energy losses to a particular ionization state, we must evaluate the integral

$$\bar{W} \sigma(E) = \int_I^{E_m} W S(E,W) dW = q_0 f_0 C_0 \int_I^{E_m} \left(\frac{I}{W} \right)^p \frac{1}{W} \left(1 - \frac{W}{E} \right)^\nu \left(\frac{W}{E} \right)^{1-\omega} dW. \quad (36)$$

For some applications it is sufficient to fit $\sigma(E)$ and $W\sigma(E)$ with the form of Eq.(27) without obtaining $S(E,W)$. As mentioned above, a good choice of parameters for Eq.(32) would be those for the allowed states, namely $\nu = 2$ and $\omega = 0.25$. The constant $C_0 f_0$ may be chosen by comparing with an experimental cross section.

If we wish to fit $\sigma(E)$ directly with Eq.(28) we can determine a good set of parameters by considering the limiting forms of Eq.(34). Near threshold we can apply the mean-value theorem for integrals to obtain

$$\sigma(E) \xrightarrow{E \rightarrow I} \frac{q_0 f_0 C_0}{I^2 \nu} \left(1 - \frac{I}{E} \right)^{\nu+1}. \quad (37)$$

That is, $\sigma(E)$ rises from threshold as the $\nu+1$ power if $S(E,W)$ rises from threshold as the ν power. Thus a power $\nu = 3$ would be the proper one to use in Eq.(28) to fit $\sigma(E)$. The asymptotic behavior will give

us the power ω . The asymptotic behavior is

$$\sigma(E) \xrightarrow{E \gg I} \frac{q_o f_o C}{(p+\omega)I} \left(\frac{I}{E}\right)^{1-\omega} \left(1 + \frac{I}{E} + \dots\right). \quad (38)$$

Thus the asymptotic power is again $1-\omega$ as it was for $S(E,W)$. Therefore we again use $\omega = 0.25$ in Eq.(28). In the same way we can represent $\bar{W}\sigma(E)$ directly in the form of Eq.(28). The parameters found useful are $\nu = 4$ and $\omega = 0.25$.

In the following chapters we will generally use the representation of $S(E,W)$ with $\nu = 2$ and $\omega = 0.25$. This representation will be found most handy for calculating secondary electron distributions. Figure 4 shows $S(E,W)$ and $\sigma(E)$ divided by $q_o f_o$.

7. Application to Atomic Oxygen

The energy level diagram of atomic oxygen is given in Herzberg and also in Figure 5. The ground state configuration is $1s^2 2s^2 2p^4$. The four $2p$ electrons can be coupled in three different ways to give three different members of the ground configuration, ^3P , ^1D and ^1S . The ^3P is the lowest in energy while the ^1D is 1.9 eV above and the ^1S is 4.17 eV above the ^3P . These three members of the ground configuration then lead to three separate ionization continua, ^4S , ^2D and ^2P , which are just the three possible combinations of the three remaining $2p$ electrons. Table 1 shows the allowed and forbidden states of atomic oxygen and the parameters for the simplified form of the cross section determined from the rules of the previous sections. The ^1D and ^1S states of the ground configuration are not included in the rules and the cross sections have been taken from Dalgarno.²⁵

Figure 4. Ionization cross section forms.

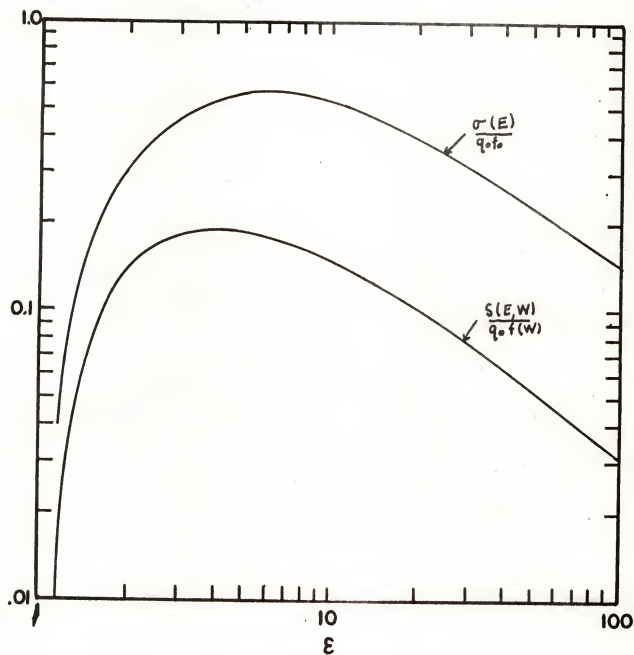


Figure 5. Energy levels of atomic oxygen. The state designation is shown along the horizontal axis and the state of the excited electron is shown alongside the level.

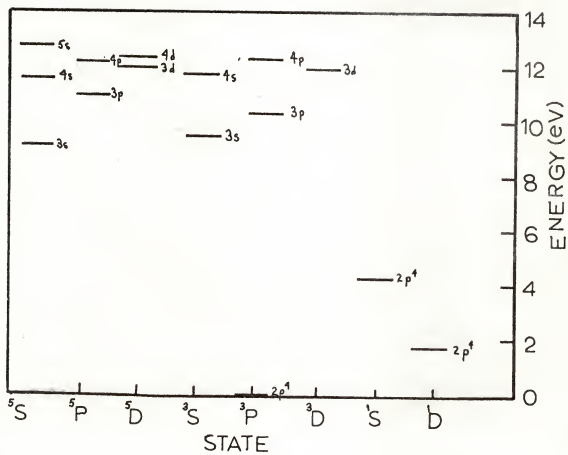


TABLE 1. Atomic Oxygen Parameters

State	Excited Electron	W_3	W_4	W_{sum}	C_{O3}	C_{O4}	$^*C_{\text{osum}}$
1) $4S$	$I = 13.6$						
$3S$	ns	9.5	11.9	13.1	.0465	.0126	.00978
$5S$	ns	9.2	11.8	13.1	.0230	.00637	.00493
$3P$	np	10.7	12.3	13.2	.0381	.00104	.00080
$5P$	np	11.0	12.4	13.2	.00313	.00852	.00658
$3D$	nd	12.1	12.8	13.3	.0150	.0063	.0081
$5D$	nd	12.1	12.8	13.3	.0254	.00692	.00535
2) $2D$	$I = 16.9$						
$3D$	ns	12.6	15.0	16.5	.0840	.0220	.0166
$1D$	ns	12.7	15.2	16.5	.0465	.0122	.0092
$3P$	np	13.7	15.5	16.5	.0061	.0016	.00121
$1P$	np	13.7	15.5	16.5	.0535	.0140	.0106
$3D$	np	14.0	15.6	16.5	.00645	.00169	.00178
$1D$	np	14.1	15.6	16.5	.060	.0157	.0119
$3F$	np	14.1	15.6	16.5	.00655	.00172	.0013
$1F$	np	14.1	15.6	16.5	.0566	.0148	.0112
$3P$	nd	15.3	16.1	16.6	.0111	.0048	.0060
$1P$	nd	15.3	16.1	16.6	.00635	.00264	.0033
$3D$	nd	15.3	16.1	16.6	.0177	.00730	.00921
$1D$	nd	15.3	16.1	16.6	.00975	.00402	.00508
$3S$	nd	15.3	16.1	16.6	.00905	.00378	.00477
$1S$	nd	15.3	16.1	16.6	.00502	.00208	.00263

TABLE 1. (Continued)

State	Excited Electron	W_3	W_4	W_{sum}	C_{O3}	C_{O4}	* C_{osum}
3)	^2P	$I = 18.5$					
^3P	ns	14.1	16.8	18.1	.0505	.0142	.0105
^1P	ns	14.4	16.9	18.1	.0316	.0081	.00597
^3S	np	15.0	17.0	18.2	.00388	.00099	.00074
^1S	np	15.0	17.0	18.2	.0338	.0087	.0064
^3P	np	15.8	17.3	18.2	.00428	.0011	.00081
^1P	np	15.8	17.3	18.2	.0374	.0096	.0071
^3D	np	15.8	17.3	18.2	.00425	.0011	.00067
^1D	np	15.9	17.3	18.2	.0381	.0098	.0072
^3P	nd	17.0	17.7	18.3	.00905	.00379	.00478
^1P	nd	17.0	17.7	18.3	.00503	.00209	.00264
^3D	nd	17.0	17.7	18.3	.0176	.0073	.0092
^1D	nd	17.0	17.7	18.3	.0145	.00602	.0076
4)							
^1S	2p			4.17			.00025
^1D	2p			1.9			.00072

* Sum denotes the sum over the higher Rydberg series members.

The cross sections for the Rydberg series of states of increasing principle quantum number n have been determined by the $1/n^3$ rule of the preceding sections. Each member of a Rydberg series is given the same shape as the first member of that series and its magnitude is set by the $1/n^3$ rule.

The breakup of the ionization cross section into the relative contributions of the ^4S , ^2D and ^2P states has been taken from Seaton.²⁶ Table 2 shows the ionization parameters.

TABLE 2. Ionization Parameters for Atomic Oxygen

State	I	C_o	ν	ω	p
^4S	13.6	0.206	2	0.25	1.5
^2D	16.9	0.206	2	0.25	1.5
^2P	18.5	0.110	2	0.25	1.5

CHAPTER III

MOLECULAR NITROGEN

1. Introduction

The purpose of this chapter is to determine a comprehensive set of inelastic electron impact cross sections for N_2 , which is an important constituent of the atmosphere of the earth and other planets. Such cross sections are needed to interpret natural phenomena, such as aurorae, airglow and lightning, as well as laboratory discharge phenomena in the air. An initial effort to assemble such a set of cross sections was made by Green and Barth¹⁸ in connection with the calculation of the intensities of auroral spectra in the ultraviolet. This work has served subsequently as a focus for a number of experimental atmospheric and laboratory studies which now make it meaningful to probe more deeply into the problem. This present work is an effort to assemble a more complete and self-consistent set of cross sections based upon more detailed studies of theoretical and experimental results.

We shall use analytical techniques which essentially are based upon the representation of angular distribution data for electron impact excitation to an excited state W in terms of the so-called generalized oscillator strength, $f(x)$, where $x = a_0^2 K^2$ where K is the magnitude of the momentum transfer. In the Born approximation region, (incident energy $E > 500$ eV), these generalized oscillator strengths

depend upon the incident energy (E) only through the dependence of x upon E. However, in the lower energy region, the generalized oscillator strength becomes an explicit function of incident energy as well. This present study is based upon the choice of analytic forms for $f(x, E)$, made in the light of intensive theoretical (Green and Dutta⁵) and phenomenological (Jusick, Watson and Green⁶) studies of atomic helium and a variety of experimental data related to helium and other substances.

2. Analytic Excitation Cross Sections

The differential excitation cross section and the total cross section may be related to Bethe's²⁷ generalized oscillator strength, which goes over to the ordinary optical oscillator strength f_0 as K , the magnitude of the momentum transfer, goes to zero. In practical treatments, it is convenient to use the dimensionless variable

$$x = a_0^2 K^2 = (2\varepsilon/x_t) [1 - \cos\theta(1 - \varepsilon^{-1})^{1/2} - (1/2\varepsilon)] \quad (1)$$

where θ is the angle of the outgoing direction with respect to the incident direction $\varepsilon = E/W$ and $x_t = W/R_e$ where R_e is the Rydberg energy. The differential cross section may be obtained from this generalized oscillator strength using

$$d\sigma/d\Omega = (4a_0^2/x_t) (1 - \varepsilon^{-1})^{1/2} f(x)/x. \quad (2)$$

The total cross section is then given by

$$\sigma = \frac{\pi a_0^2 (2R_e)^2}{W^2} \frac{W}{E} \int_{x_0}^{x_u} \frac{f(x)}{x} dx \quad (3)$$

where x_u and x_λ are the square of the momentum changes corresponding to backward ($\theta = \pi$) and forward ($\theta = 0$) scattering, respectively. It should be noted that x_u and x_λ both go to x_t as $E \rightarrow W$, so that the cross section vanishes at the threshold if these exact limits are used.

Quantum mechanical considerations may be brought to bear on the determination of $f(x)$ if good wave functions are available for the states in question. Today we are almost in a position to carry out such calculations for atoms. However, undoubtedly it will be some time before such direct theoretical calculations can be carried out for atmospheric molecules. Fortunately, however, it is possible to proceed phenomenologically by taking advantage of experimental data which are more available for molecules than for atoms. In particular, an extensive series of experimental curves of $f(x)$ by Lassettre, et al.⁸⁻¹⁴ show that many $f(x)$ curves have a simple behavior which may be conveniently represented by an analytic function of the form

$$f(x) = f_0 \exp -\alpha \xi + f_1 \xi \exp -\beta \xi \quad (4)$$

where $\xi = x/x_t$ and f_0 , α , f_1 and β represent adjustable parameters. The same functional form also describes the theoretical oscillator strengths for helium very well.

If a limited range of differential cross section data is available for one or two energies, these data may be converted to an experimental $f(x)$ function using Eqs.(1) and (2). If the experimental function is fitted by Eq.(4), then the analytic form serves as a reasonable basis for extrapolating $f(x)$ outside the region of measurements. Hence, using Eqs.(1) and (2) we may evaluate the differential cross section

at any angle and energy. Furthermore, Eq.(5) may then be integrated analytically to obtain the total cross section in terms of the parameters of the analytic form of $f(x)$.

These results apply only in the region of the Born approximation. To deal with lower energies for light substances, we use a phenomenologically distorted $f(x)$ which is then an explicit function of E as well. The forms chosen have been based upon the studies of helium by Green and Dutta⁵ and Jusick, Watson and Green⁶ in which they made use of the considerable experimental data, particularly those of St. John, et al.,²⁸ and also upon old low energy angular distribution data on N_2 by Mohr and Nicholl²⁹ and McMillen.³⁰

This "distorted" oscillator strength which we will use for light substances has the form

$$f(x,E) = (1-\epsilon^{-1})^\tau f_B(\xi) + (C/\gamma)(1-\epsilon^{-1})^\delta \epsilon^{-m} \xi \exp(-\gamma \xi) \quad (5)$$

where τ , C , γ , m and δ are additional low energy parameters. At high energies $f(x,E) \rightarrow f_B(x)$. Using $f(x,E)$ in Eq.(3), the total cross section is

$$\begin{aligned} \sigma(E) = & \frac{q_0}{W} \frac{W}{E} f_0 D(\tau, 0) \left[E_1 \left(\alpha \frac{x_l}{x_t} \right) - E_1 \left(\alpha \frac{x_u}{x_t} \right) \right] \\ & + \frac{f_1}{\beta} D(\tau, 0) \left[\exp \left(-\beta \frac{x_l}{x_t} \right) - \exp \left(-\beta \frac{x_u}{x_t} \right) \right] \\ & + \frac{f_l}{\gamma} D(\delta, m) \left[\exp \left(-\gamma \frac{x_l}{x_u} \right) - \exp \left(-\gamma \frac{x_u}{x_t} \right) \right] \end{aligned} \quad (6)$$

where $q_0 = 6.513 \times 10^{-14} \text{ cm}^2 \text{ eV}^2$

$$\frac{x_l}{x_t} = \frac{E}{W} (1 - \sqrt{1 - \frac{W}{E}})^2 \quad \frac{x_u}{x_t} = \frac{E}{W} (1 + \sqrt{1 - \frac{W}{E}})^2 \quad (7)$$

and

$$D(\nu, \Omega) = [1 - (W/E)]^\nu (W/E)^\Omega \quad (8)$$

and $E_1(2)$ is the first exponential integral. This function may be dealt with conveniently and accurately using approximate formulas given by Gautschi and Cahill.³¹ Thus, Eq.(6) constitutes a universal cross section formula for any transition in light substances which gives the cross section at any energy E depending upon the high energy parameters f_0 , α , f_1 , β , and five low energy parameters τ , C , γ , m and δ .

While this system may appear to be quite cumbersome, nevertheless, in conjunction with a simple computer program it provides a very practical means for bringing accumulated theoretical and experimental experience and fragmentary experimental data to bear upon the generation of $\sigma(E)$ for many transitions. In the first place, the most important parameter f_0 is frequently known from optical data, from theory, or from phenomenological rules. In the second place, the high energy shape parameters α , $\kappa = f_1/f_0$ and β , appear to vary over rather narrow limits and to remain constant for Rydberg series. Thus, if the shape parameters of one member are known, we may apply them to all members. Furthermore, studies of helium data suggest that for most purposes we may set κ to zero. In the third place, the total cross sections are not very sensitive to the low energy parameters. Hence, in the absence of additional detailed evidence we may use low energy parameters based upon the corresponding types of transitions in helium. Accordingly, at this time detailed problem is simply one

of fixing two or four parameters, the most important of which can often be deduced from optical data.

3. Allowed Transitions

To evaluate the parameters f_o , α , κ and β for allowed transitions we have used experimental data of Lassetre and Krasnow⁹ and Silverman and Lassetre⁸ who have measured generalized differential oscillator strengths of N_2 at energy losses ranging from 9.1 to 82 eV and at momentum transfers ranging from $x = 0.1$ to 2.0. We have identified the low energy losses with particular discrete electronic states of N_2 and N_2^+ , using the reports of Gilmore,³² Mullikan,³³ and Cook and Ogawa.³⁴ We also compare the optical oscillator strengths with those obtained from the data of Huffman, Tanaka, and Larrabee³⁵ with those extracted from our forms of the generalized oscillator strengths. The energy level diagram of N_2 is shown in Figure 6.

Silverman and Lassetre⁸ have obtained generalized differential oscillator strengths for two peaks in the electron impact spectrum of N_2 at 12.85 and 14.0 eV above the ground state ($X^1\Sigma_g^+$). There are several states contributing to the electron impact spectrum at these energy losses, including a large contribution due to some of the lower members of Rydberg series leading to the ionization continua. The parameters obtained by fitting the differential oscillator strengths of the entire peaks are given in Table 3. In order to determine how much of the cross sections of these peaks is due to Rydberg series, we need a method of determining the magnitude of the Rydberg series from known quantities. This can be most easily accomplished by considering

Figure 6. Energy levels of N_2 .

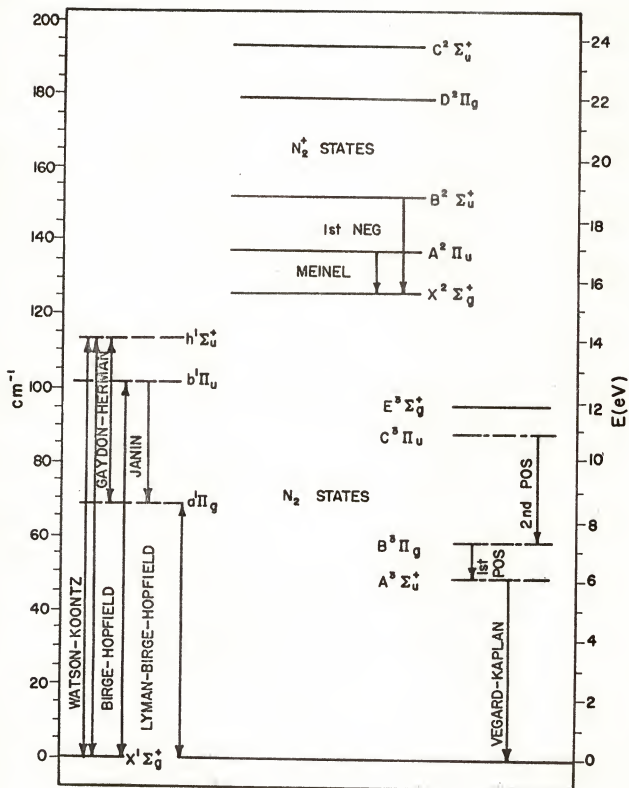


TABLE 3. N_2 Allowed Parameters

12.85 and 14.0 Peaks

State	W	f_0	x_t	α	f_1	β
Total						
12.85 Peak	12.85	1.09	0.945	3.2	0.172	0.690
$b^1\pi_u$	12.85	0.184	0.945	3.2	0.172	0.690
$R_x(3)$	13.0	0.556	0.955	3.0	0.	0.
$R_A(3)$	13.17	0.191	0.969	3.0	0.	0.
Total						
14.0 Peak	14.0	0.671	1.028	2.26	0.0504	0.344
$h^1\Sigma_u^+$	14.0	0.183	1.028	2.26	0.0504	0.344
$R_x(4)$	14.4	0.189	1.060	3.0	0.	0.
$R_c(3)$	14.0	0.275	1.029	3.0	0.	0.

TABLE 3. (Continued)

STATE	c	δ	m	τ	γ	C_0	ν	ω
Total								
12.85 Peak	0.100	0.5	2.0	2.0	0.17	1.60	3	0.25
$b^1\pi_u$	0.017	0.5	2.0	2.0	0.17	0.444	3	0.25
$R_x(3)$	0.051	0.5	2.0	2.0	0.17	0.856	3	0.25
$R_A(3)$	0.018	0.5	2.0	2.0	0.17	0.320	3	0.25
Total								
14.0 Peak	0.061	0.5	2.0	2.0	0.17	1.052	3	0.25
$h^1\Sigma_u^+$	0.0167	0.5	2.0	2.0	0.17	0.391	3	0.25
$R_x(4)$	0.0173	0.5	2.0	2.0	0.17	0.280	3	0.25
$R_c(3)$	0.0251	0.5	2.0	2.0	0.17	0.418	3	0.25

the ionization limit to which each series converges. Table 4 shows the Rydberg energy levels to each ionization limit taken from Ogawa³⁶ and Wallace.³⁷ The series leading to the $D^2\pi_g$ and $C^2\Sigma_u^+$ ionization continua have not been observed and are thus somewhat arbitrarily placed to correspond to the peaks in Skerbele and Lassettre's¹¹ impact spectrum. It is seen that the $n = 3$ member of the series leading to the $X^2\Sigma_g^+$ continuum [denoted by $R_x(3)$] and the $n = 3$ member of the series leading to the $A^2\Pi_u$ continuum lie under the 12.85 peak in the impact spectrum. Also, the $n = 4$ member of the $X^2\Sigma_g^+$ series and the $n = 3$ member of the $C^2\Sigma_u^+$ series fall under the 14.0 peak. The magnitudes of these levels along with the magnitudes of the remaining Rydberg series levels are determined from the oscillator strengths in the respective continuum to which each series converges.

In the next section we will obtain expressions for the optical oscillator strength per unit energy loss, df/dW , for each ionization continuum. The value of df/dW at $W = I$ will be equal to the value of the optical oscillator strength per unit energy interval in the Rydberg series as $n \rightarrow \infty$. If the optical oscillator strength within a Rydberg series is given by

$$f_n = \frac{c}{n^{*3}} \quad (9)$$

where n^* is the effective quantum number, then the constant c is given by

$$c = 27.2 \left. \frac{df}{dW} \right|_{W=I} \quad (10)$$

In order to determine $df/dW|_{W=I}$, we must first determine the relative sizes of the continua for N_2 . This is done by considering

TABLE 4. Rydberg Series Levels and Oscillator Strengths

IONIZATION LIMIT	n	n [*]	E _n	f _n
$X^2\Sigma_g^+$	3	2.3	13.0	.556
	4	3.3	14.4	.189
	sum		15.1	.236
$A^2\Pi_u$	3	1.96	13.17	.191
	4	2.96	15.2	.055
	sum		16.2	.0567
$B^2\Sigma_u^+$	3	2.13	15.75	.0654
	4	3.13	17.3	.0187
	sum		18.2	.0219
$D^2\Pi_g$	3	1.47	15.7	.104
	4	2.47	19.8	.0315
	sum		21.3	.0250
$C^2\Sigma_u^+$	3	2.2	14.0	.275
	4	3.2	20.8	.0448
	sum		22.6	.0280

the 0° electron impact spectrum of Skerbele and Lassetre.¹¹ This spectrum is made up of peaks due to Rydberg series superimposed over the direct ionization continua. Figure 7 shows a typical Rydberg series impact spectrum along with its ionization continuum. By adjusting the relative sizes of the continua and their attached Rydberg series, we obtain an approximate fit to the impact spectrum. For this purpose a line width of the Rydberg members of approximately 1/2 volt has been used. The fit obtained is shown in Figure 8 and the relative sizes of the continua are given in Table 5. After the relative sizes of the df/dW are determined, the absolute magnitudes can be determined from the data of Silverman and Lassetre⁸ at high energy loss. Then the f_n for all of the Rydberg levels is determined. The parameters for the shape of the Rydberg levels are, in the absence of any data, assumed to be the same as those given for helium allowed transitions by Jusick, Watson, and Green. These are shown in Table 3. The oscillator strengths of all of the Rydberg series levels are shown in Table 4. These Rydberg members are subtracted from the total cross section under the peak and the remainder is identified with the $b^1\pi_u$ for the 12.85 peak and the $h^1\Sigma_u^+$ for the 14.0 peak. There are still many levels included in this remainder but the identified states are probably the most important. There may also be some forbidden states mixed in as indicated by the f_1 term. The cross sections are shown in Figures 9 and 10.

Some of the Rydberg series levels to the higher ionization continua have energies which are above the lowest ionization threshold and can therefore autoionize. The branching ratio for autoionization was roughly estimated from Cook and Ogawa³⁴ to be 50%. On this basis, the

Figure 7. Impact spectrum for a typical Rydberg series and ionization continuum.

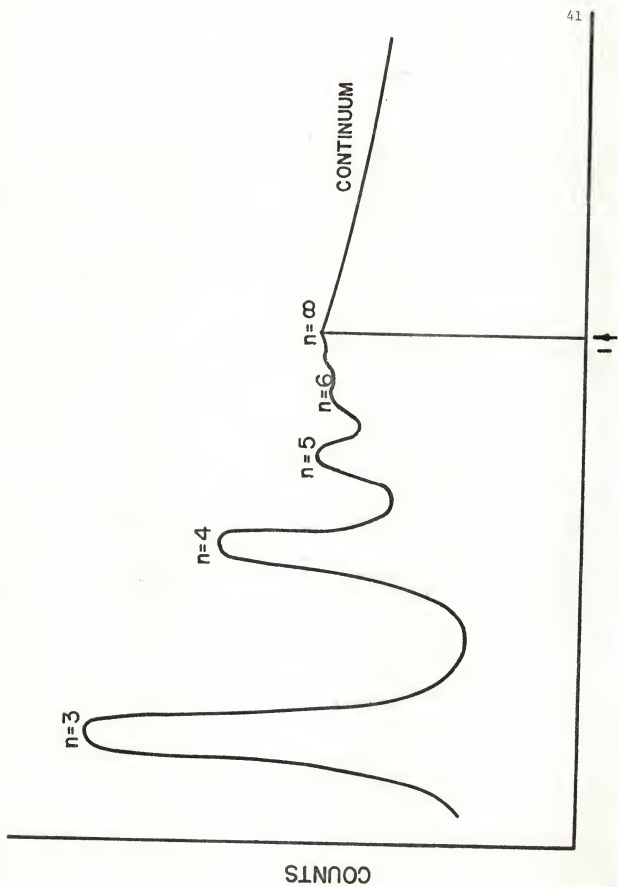


Figure 8. Zero angle impact spectrum of N_2 .

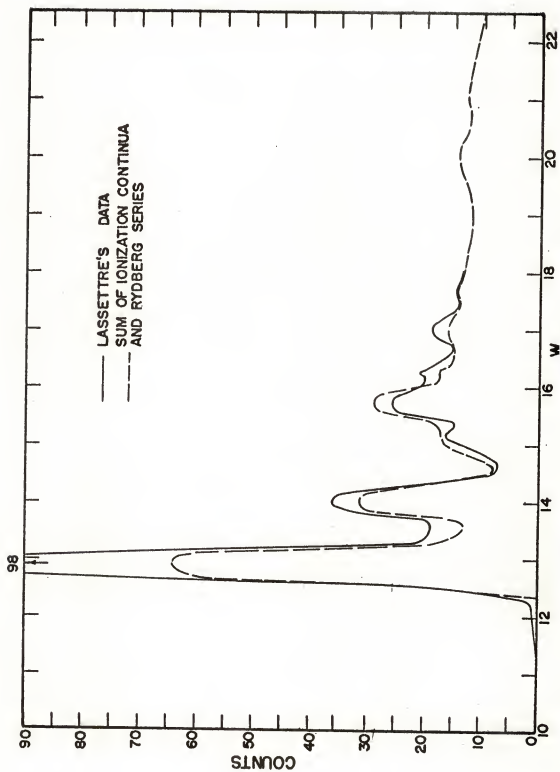


TABLE 5. Relative Sizes of Ionization Continua

Continuum State	Threshold (eV)	Size (%)
$X^2\Sigma_g^+$	15.58	70
$A^2\Pi_u$	16.73	15
$B^2\Sigma_u^+$	18.75	5
$D^2\Pi_g$	22.0	5
$C^2\Sigma_u^+$	23.6	5

Figure 9. Allowed generalized oscillator strengths
for N_2 .

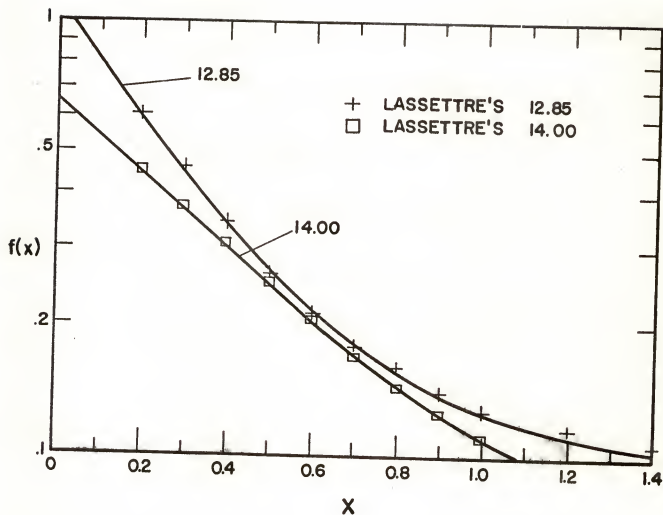
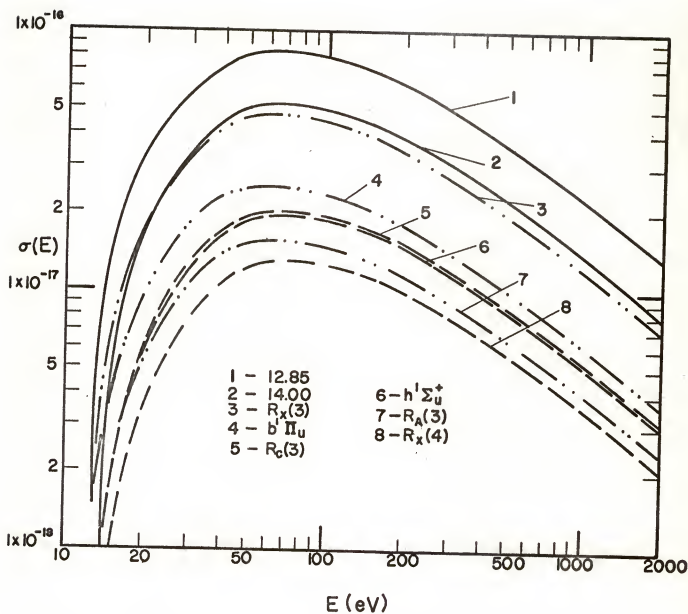


Figure 10. Allowed cross sections for N_2 - 12.85 and 14.0 peaks. Solid curves correspond to cross section for entire 12.85 and 14.0 peaks in impact spectrum, dashed curves correspond to cross sections of component parts of 14.0 peak, and dash-dot-dash curves correspond to cross sections of component parts of 12.85 peak.



autoionization cross sections summed over the members of each series were obtained and are shown in Figure 11. These are then to be added to the direct ionization continuum to obtain a comparison with measured total ionization cross sections.

4. Forbidden Transitions

We have considered four forbidden transitions (forbidden in the optical sense by electric dipole radiation) in our analysis of N_2 . Lassette and Krasnow⁹ have obtained a generalized differential oscillator strength at an energy loss of 9.1 eV, which is identified with the $a^1\pi_g$ state of N_2 . They have identified it as 87% magnetic dipole transition and 13% electric quadrupole transition. Since the optical oscillator strengths are known to be extremely small for forbidden transitions, we have used the same functional form as given by Eqs. (4) and (5), however, with $f_0 = 0$. Parameters in the energy dependent term were taken from the study of forbidden helium transitions.

Magnitudes for the three triplet states $A^3\Sigma_u^+$, $B^3\pi_g$ and $C^3\pi_u$ at 6.14, 7.3 and 11.03 eV were obtained from the cross sections of Green and Barth.¹⁸ Here, in the absence of generalized oscillator strength data, β was taken as 3. The coefficient f_1 was then obtained from the previously quoted work.

The modified cross sections and the values of the parameters are shown in Figure 12 and Table 6, respectively.

5. Ionization Continuum

Having obtained the relative contributions of the various continua to the total oscillator strength, we then fit the total df/dW of

Figure 11. Allowed cross sections - higher Rydberg series members.

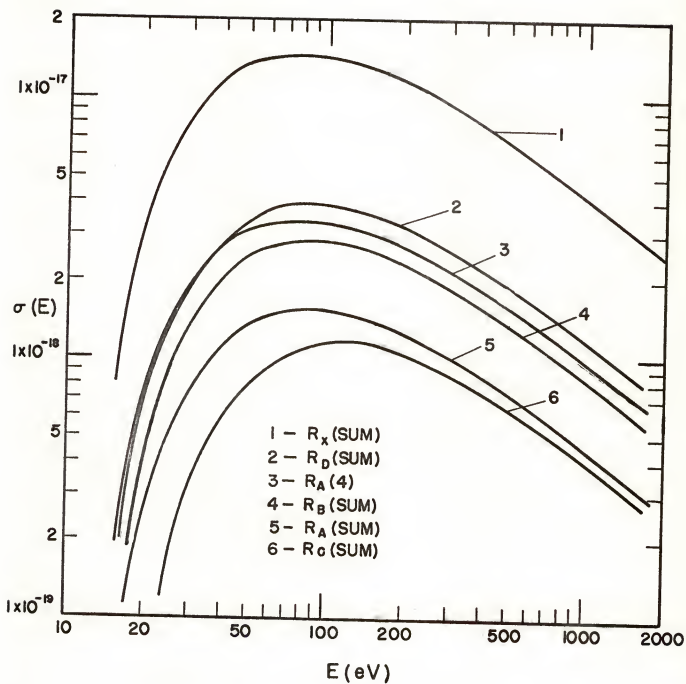


Figure 12. Forbidden cross sections.

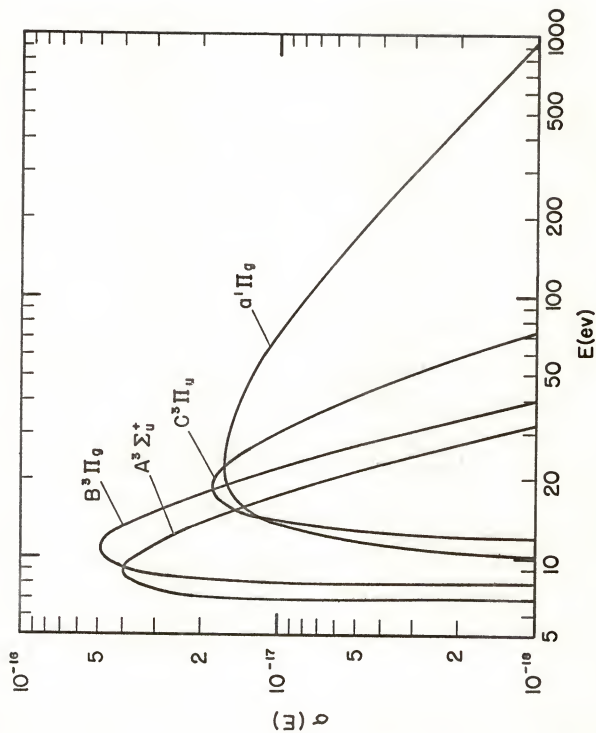


TABLE 6. N_2 Parameters for Forbidden States

STATE	W	f_o	x_t	α	f_1	β
$A^3\Sigma_u^+$	6.14	0	0.493	0	0	0
$B^3\Pi_g$	7.3	0	0.544	0	0	0
$a^1\Pi_g$	9.1	0	0.669	0	0.143	1.06
$C^2\Pi_u$	11.03	0	0.823	0	0	0

TABLE 6. (Continued)

STATE	c	δ	m	τ	γ	C_o	ν	ω
$A^3\Sigma_u^+$	0.237	1.3	3.5	2.0	0.17	0.609	1.5	-3
$B^3\Pi_g$	0.423	1.3	3.5	2.0	0.17	1.08	1.5	-3
$a^1\Pi_g$	0.174	2.3	3.5	2.0	0.17	0.140	2.0	0
$C^2\Pi_u$	0.284	1.6	2.5	2.0	0.17	0.541	1.5	-2

Silverman and Lassette⁸ at energy losses greater than the excitation energy of the highest contributing state ($C^2\pi_u$) in N_2^+ . This was done in order to separate out the contribution due to excitation of members of the Rydberg series which can autoionize. The form chosen to fit the ionization data is (Jusick, Watson and Green⁶)

$$\frac{d^2 f}{dW dx} = F_0 + F_1 + F_2 + F_\ell \quad (11)$$

where

$$F_0 = B_0 (w + a_1)^{-n_1} \exp -\alpha_0 x/x_t \quad (12)$$

$$F_1 = B_1 w^{n_5} [w - 1/w]^{n_4} (x e a_1 / x_t) \exp -\alpha_1 x/x_t \quad (13)$$

$$F_2 = B_2 w^{-n_2} [w - 1/w]^{n_3} [x e / x_t] \exp -\alpha_2 x \quad (14)$$

and

$$F_\ell = B_3 (w/E)^m [1 - (w/E)]^\delta (x/x_t) \exp -\alpha_3 x/x_t \quad (15)$$

where $w = W/I$. This form for the continuum has been arrived at after a rather elaborate chain of logic. The starting point was the quite complex Massey and Mohr³⁸ expression for the hydrogenic continuum which is based upon Sommerfeld hydrogenic functions. This "Bethe Surface" could be approximated very well by a sum of the first three terms, a decomposition which is rather convenient if one then wishes to distort the theoretical surface to fit experimental data. Such a distortion was made to helium data which led to the particular dependences upon w given in Eqs.(11) through (13). The fact that this form

can be used to satisfy sum rule and that at high x a peak occurs at $x = x_t$ were important in the selection of this form, in particular the F_2 term.

In the case of N_2 , as in He, the data available were sufficient to fix the parameters in F_0 and F_1 . Therefore, F_2 was chosen a) to satisfy the sum rule, and b) to match the high energy ionization data. The quantity F_ℓ is a low energy modification based upon helium studies. The parameters of the fits are given in Table 7.

The above information can be used to obtain the direct ionization cross section by the formula

$$\sigma(E) = \int_I^{(E+I)/2} \int_{x_\ell}^x \frac{f(x, W, E)}{x} dx dW. \quad (16)$$

These parameters are chosen not only to fit the differential oscillator strength, $d^2f/dWdx$, but also the Bethe sum rule. Since the data of Silverman and Lassetre are taken over a limited energy loss range, one can adjust the high behavior to conform to the sum rule. This was done to a precision of 15%. Having obtained the direct ionization component, we can now compute the total ionization by the equation

$$\sigma_T = \beta \sigma_R + \sigma_{DI} \quad (17)$$

where σ_T is the total ionization cross section, σ_R is the Rydberg series excitation cross section, β is the branching ratio ($\beta = .5$) and σ_{DI} is the direct ionization cross section. A comparison of the results is shown in Figure 13. We also note that the autoionizing component is, approximately, 5% of the total. This is due to the

TABLE 7. N_2 Ionization Parameters

State	I	B_0	B_1	B_2	B_3	m	τ	δ	α_3
$X^2\Sigma_g^+$	15.58	2.48	51.7	738	19.3	2.0	2.0	3.0	0.17
$A^2\Pi_u^+$	16.73	0.526	11.1	158	4.09	2.0	2.0	3.0	0.17
$B^2\Sigma_u^+$	18.75	0.175	3.70	60.8	1.36	2.0	2.0	3.0	0.17
$D^2\Pi_g$	22.0	0.175	3.70	60.8	1.36	2.0	2.0	3.0	0.17
$C^2\Sigma_u^+$	23.6	0.175	3.70	60.8	1.36	2.0	2.0	3.0	0.17

TABLE 7. (Continued)

State	C_0	ν	ω	p
$X^2\Sigma_g^+$	.545	2	0.25	1.5
$A^2\Pi_u^+$	.143	2	0.25	1.5
$B^2\Sigma_u^+$	.051	2	0.25	1.5
$D^2\Pi_g$	.060	2	0.25	1.5
$C^2\Sigma_u^+$	.064	2	0.25	1.5

All States

$a_1 = 1.75$

$\alpha_0 = 1.75$

$n_1 = 2.25$

$\alpha_1 = 3.5$

$n_2 = 3.6$

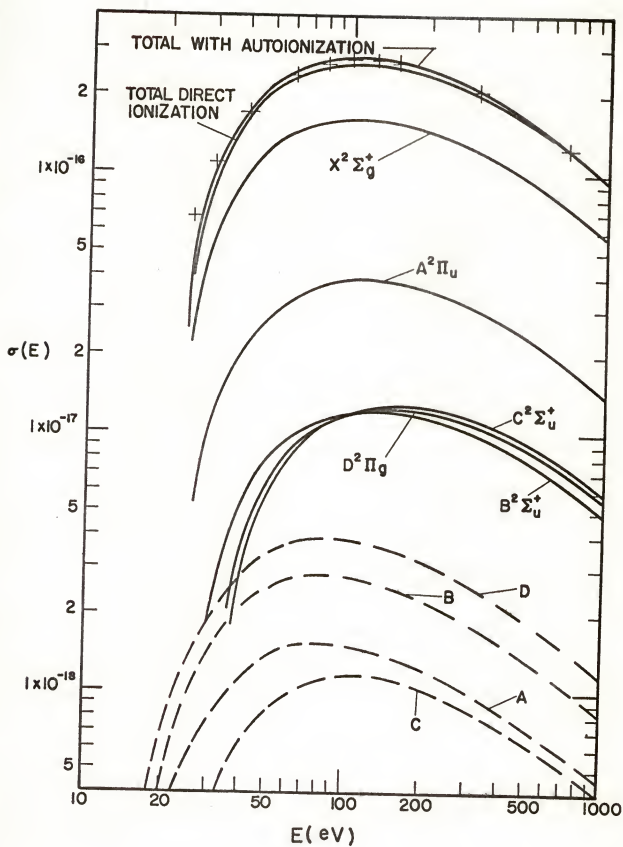
$\alpha_2 = 1.0$

$n_3 = 12.0$

$n_4 = 6.0$

$n_5 = 4.0$

Figure 13. Ionization cross sections. Solid curves are direct ionization, dashed curves are auto-ionization, and crosses are total ionization data of Golden and Rapp.⁵⁴



particular structure of N_2 which gives most of the strength of the ionizing transitions (70%) to the ground state of N_2^+ , which then is energetically unable to autoionize. The situation is far different in O_2 .

6. Franck-Condon Factors and Vibrational Excitation

We have not attempted in this chapter to decompose our electronic excitation cross sections into their vibrational subcomponents. However, if Franck-Condon factors are available, the decomposition is straightforward. For this work it is more convenient to use the simpler functional forms of the preceding section. Then the cross sections from the ground vibrational member of the ground electronic state to the v^{th} vibrational member of the upper electronic state is

$$\sigma_v(E) = q_v \sigma_T(E, W + \Delta) \quad (18)$$

where Δ is the energy difference between the 0^{th} and v^{th} vibrational substates of the upper electronic state and q_v is the Franck-Condon factor.

Vibrational excitation enters into the electron impact cross section of N_2 in an entirely different way. There appears in the total collision cross section of nitrogen, a rather large peak centered at about 2.4 eV which is approximately a factor of three larger than the general background. This has been interpreted by Schulz,³⁹ Herzberg and Mandl⁴⁰ and Chen⁴¹ to be due to compound molecule formation of N_2^- , followed by decay to the ground states of the $X^1\Sigma_g$ of N_2 . Thus the broad peak in the total collision cross section is the sum

of vibrational excitation and compound elastic scattering cross sections. By the nature of the process, the cross section only becomes significant when the kinetic energy of the incident electron is sufficient to resonate with the ground state of N_2^- or the higher vibrational states of N_2^- which occur at a spacing of approximately 0.25 eV. The decay can proceed downward to either the ground vibrational state of N_2 or various energetically allowed vibrational states which are spaced at about 0.20 eV.

Herzenberg and Mandl and Chen have presented mathematical formalism for dealing with vibrational excitation of molecules involving resonance with negative ion states. Their work has been applied to the experimental data of Schulz. As yet, the theoretical results have only a qualitative similarity to the rather incomplete experimental results even after adjustment of absolute magnitudes. In view of this we will not attempt to deal with this problem in detail. However, we may simulate the average effect of compound molecule formation followed by vibrational excitation of N_2 by assuming there is an effective cross section given by the Green-Barth form with the parameters, $W = 1.4$ eV, $C_0 = 1.3 \times 10^8$, $v = 16$ and $w = -15$. This representation should be adequate to allow for vibrational excitation in energy loss calculations.

This work is an attempt to bring all the known experimental and theoretical information on N_2 as well as a knowledge of systematic trends of electron impact cross sections to bear upon the determination of as complete a set of impact cross sections as can be obtained at this time. The final results have been fitted to the analytic

forms of Green and Barth¹⁸ and the parameters are shown in the last three columns of Tables 4, 6 and 7. The intended applications are primarily to energy loss problems in the upper atmosphere and calculation of secondary electron and tertiary electron distributions arising in connection with the aurora and the airglow problems, which will be discussed in Chapters V - VIII of this dissertation.

CHAPTER IV

MOLECULAR OXYGEN

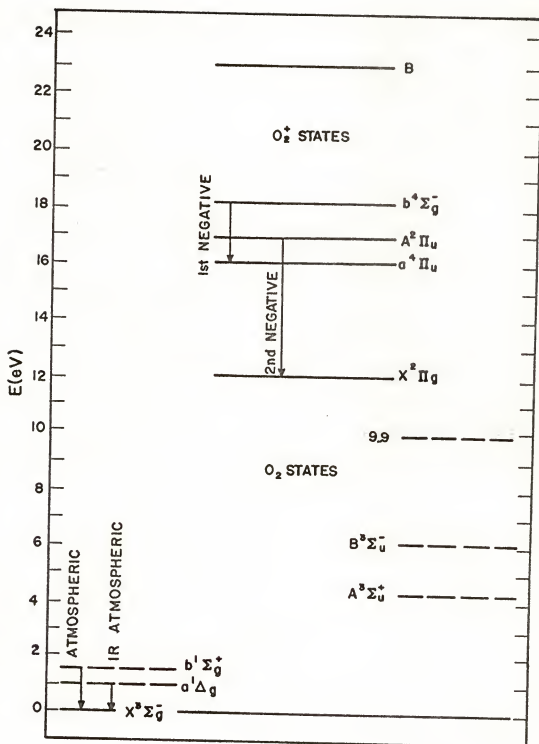
1. Introduction

The purpose of this chapter is to determine a comprehensive set of inelastic electron impact cross sections for O_2 . The methods used are the same as in Chapter III, and we will only point out the significant differences between O_2 and N_2 in this chapter. The report of Gilmore,³² along with the optical absorption data of Watanabe, et al.,⁴² Lee⁴³ and Cook and Metzger,⁴⁴ was used to identify the peaks in the impact spectrum of Silverman and Lassettre.^{15,16} We have identified three forbidden transitions at 0.98, 1.64, and 4.5 eV as $a^1\Delta_g$, $b^1\Sigma_g^+$, and $A^3\Sigma_u^+$ respectively. We have used the two allowed transitions of Silverman and Lassettre^{15,16} at 8.4 and 9.9 eV. They identified the 8.4 eV transition as the $B^3\Sigma_u^-$ Schumann-Runge dissociation continuum. They did not identify the 9.9 eV transition and it probably involves many unresolved states. Five ionizing transitions at 12.1, 16.1, 16.9, 18.2 and 23.0 eV were identified as $X^2\Pi_g$, $a^4\Pi_u$, $A^2\Pi_u$, $b^4\Sigma_g^-$ and B. The fifth ionization transition at 23.0 is probably a combination of transitions ranging from 22 to 24 eV. The energy levels of O_2 are shown in Figure 14.

2. Allowed Transitions

Lassettre, et al.¹⁷ have obtained generalized oscillator strengths for two peaks in the electron impact spectrum of O_2 at 8.4 and 9.9 eV

Figure 14. Energy levels of O_2 .



above the ground state ($X^3\Sigma_g^-$). As was the case in N_2 , there are probably several states contributing to the peaks at these energy losses. For O_2 we have been able to identify only the $n = 3$ member of the Rydberg series to the $X^2\Pi_g$ ionization limit as being part of the 8.4 eV peak. Since it is more than 90% of the peak we must assume that it is the $B^3\Sigma_u^-$ state.

The Rydberg series cross sections have been determined in the same way as in N_2 , that is, the oscillator strengths were assumed to follow a $1/n^{*3}$ rule, where n^* is the effective quantum number, and the magnitude was set from df/dW at the ionization limit. The impact spectrum obtained in this way is shown in Figure 15 along with the data of Silverman and Lassetre. It is seen that we obtain semi-quantitative agreement with data. The percentage of the cross section into each ionization state is shown in Table 10.

Figure 16 shows the oscillator strengths of Silverman and Lassetre along with the fit obtained with Eq.(5) of Chapter III. Table 8 gives the parameters used to obtain the fits to these total peaks along with the break up of the 8.4 peak into the $n = 3$ member of the $X^2\Pi_g$ Rydberg series and the remainder. The cross sections obtained with these parameters by Eq.(6) of Chapter III are shown in Figure 17. The energy levels and oscillator strengths for the remainder of the Rydberg series are given in Table 9. Just as in N_2 , the parameters for the shape of the Rydberg cross sections are, in the absence of any data, assumed to be the same as those given for helium by Jusick, Watson and Green.⁶

Note that most of the higher Rydberg members lie above the first ionization continuum and can therefore autoionize. A 50% branching

Figure 15. Zero angle impact spectrum of O_2 .

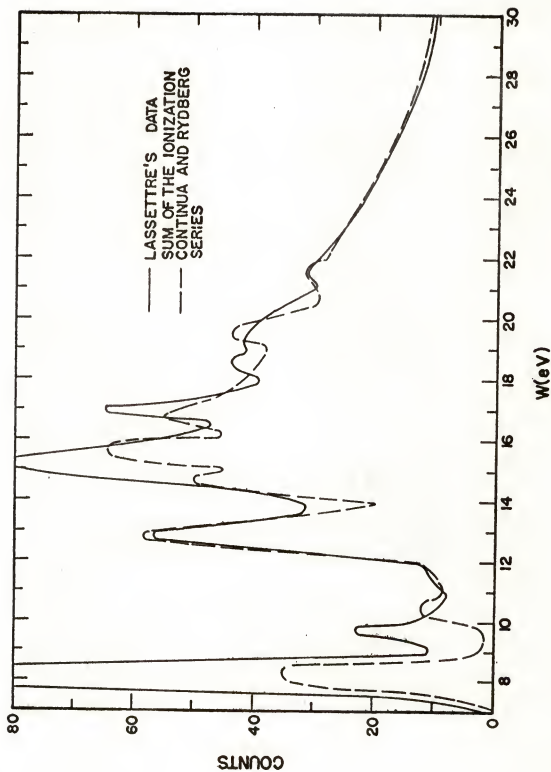


TABLE 8. O_2 Allowed Parameters

8.4 and 9.9 eV Peaks

State	W	f_o	x_t	α	f_1	β
Total						
8.4 Peak	8.4	0.230	0.617	1.20	8.30×10^{-3}	0.102
$R_x(3)$	8.4	0.215	0.617	1.20	0.	0.
Remainder	8.4	0.015	0.617	1.20	8.30×10^{-3}	0.102
Total						
9.9 Peak	9.9	0.0253	0.728	0.43	0.	0.

TABLE 8. (Continued)

State	c	δ	m	τ	γ	C_o	ν	ω
Total								
8.4 Peak	2.09×10^{-2}	0.5	2.0	2.0	0.17	.520	3.0	0.20
$R_x(3)$	1.95×10^{-2}	0.5	2.0	2.0	0.17	.455	3.0	0.20
Remainder	1.36×10^{-3}	0.5	2.0	2.0	0.17	.0693	2.0	0.20
Total								
9.9 Peak	2.30×10^{-3}	0.5	2.0	2.0	0.17	.0477	2.5	0.20

TABLE 9. O_2 Rydberg Series

Ionization Limit	n	n^*	E_n	f_n
$X^2\pi_g$	3	1.92	8.4	.215
	4	2.92	10.5	.061
	Sum		11.6	.050
$a^4\pi_u$	3	2.0	12.7	.432
	4	3.0	14.6	.115
	Sum		15.6	.122
$A^2\pi_u$	3	1.93	13.2	.432
	4	2.93	15.3	.123
	Sum		16.2	.153
$b^4\Sigma_g^-$	3	2.31	15.7	.193
	4	3.31	16.9	.0653
	Sum		17.7	.0844
$B(^4\Sigma_u^- ^2\Sigma_g^-)$	3	2.0	19.6	.129
	4	3.0	21.5	.0384
	Sum		22.5	.0365

TABLE 10. O_2 Relative Sizes of Ionization Continua

Continuum State	Threshold (eV)	Size (%)
$X^2\Pi_g$	12.1	17
$a^4\Pi_u$	16.1	37
$A^2\Pi_u$	16.9	22
$b^4\Sigma_g^-$	18.2	15
$B(^4\Sigma_u^-, ^2\Sigma_g^-)$	23.0	9

Figure 16. Allowed generalized oscillator strengths
of O_2 .

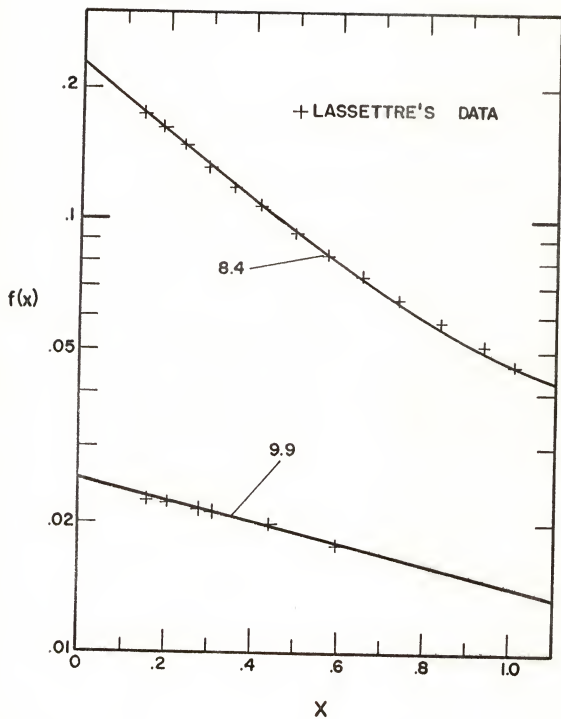
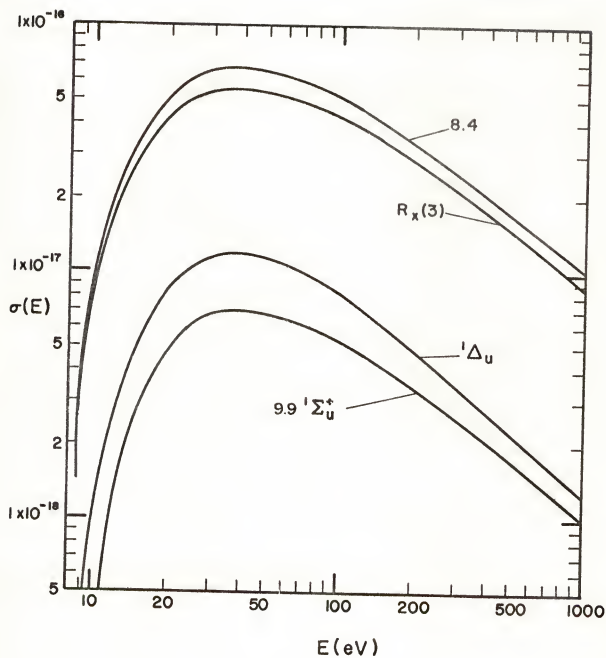


Figure 17. Allowed cross sections - 8.4 and 9.9 eV peaks.



ratio was assumed and the resulting autoionization cross sections are shown in Figure 18. Figure 17 shows the remaining 50% of the Rydberg cross sections which result in discrete excitation.

3. Forbidden Transitions

We have considered three forbidden transitions in our analysis of O_2 . They have been identified from the report of Gilmore³² along with the optical absorption data of Watanabe, *et al.*,⁴² Lee⁴³ and Cook and Metzger⁴⁴ as $a^1\Delta_g$ at 0.98 eV, $b^1\Sigma_g^+$ at 1.64 eV, and $A^3\Sigma_u^+$ at 4.5 eV. These transitions are all of the same type as the $9.1\text{ eV } a^1\pi_g$ transition in N_2 . The parameters used are shown in Table 11 and the resulting cross sections in Figure 19.

4. Ionization Continuum

Having obtained the relative contributions of the various continua to the total oscillator strength from the electron impact spectrum, we then fit the total df/dW of Silverman and Lassetre^{15,16} at energy losses greater than the excitation energy of the highest contributing state in O_2^+ . The form chosen was the same as for N_2 given in Eqs.(11) through (15) of Chapter III. The direct ionization cross section is then given by Eq.(16) of Chapter III, and the total direct plus autoionization by Eq.(17) of Chapter III. The parameters and cross sections are shown in Table 12 and Figure 20, respectively. The large contribution to autoionization compared to N_2 is due to most of the continuum oscillator strength being assigned to the 16.1 and 16.9 eV states, whose Rydberg series lie above the first ionization state at 12.1 eV. The parameters to the simplified forms of Green and Barth¹⁸

Figure 18. Allowed cross sections - higher Rydberg series members.

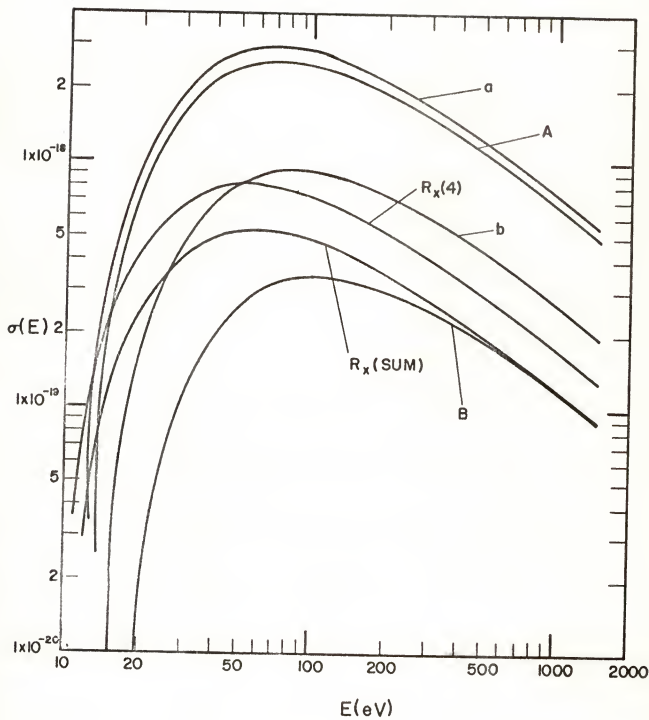


TABLE 11. O_2 Forbidden Parameters

State	W	f_o	x_t	α	f_1	β
$a^1\Delta_g$	0.98	0	0.0721	0	3.07×10^{-5}	3.0
$b^1\Sigma_g^+$	1.64	0	0.121	0	5.12×10^{-5}	3.0
$A^3\Sigma_u^+$	4.5	0	0.331	0	1.15×10^{-1}	3.0

TABLE 11. (Continued)

State	c	δ	m	τ	γ	C_o	ν	ω
$a^1\Delta_g$	$3.73 \cdot 10^{-5}$	2.3	3.5	2.0	0.17	$4.90 \cdot 10^{-5}$	1.5	0
$b^1\Sigma_g^+$	$6.22 \cdot 10^{-5}$	2.3	3.5	2.0	0.17	$5.38 \cdot 10^{-5}$	1.5	0
$A^3\Sigma_u^+$	$1.39 \cdot 10^{-1}$	2.3	3.5	2.0	0.17	$3.11 \cdot 10^{-2}$	1.5	0

Figure 19. Forbidden cross sections.

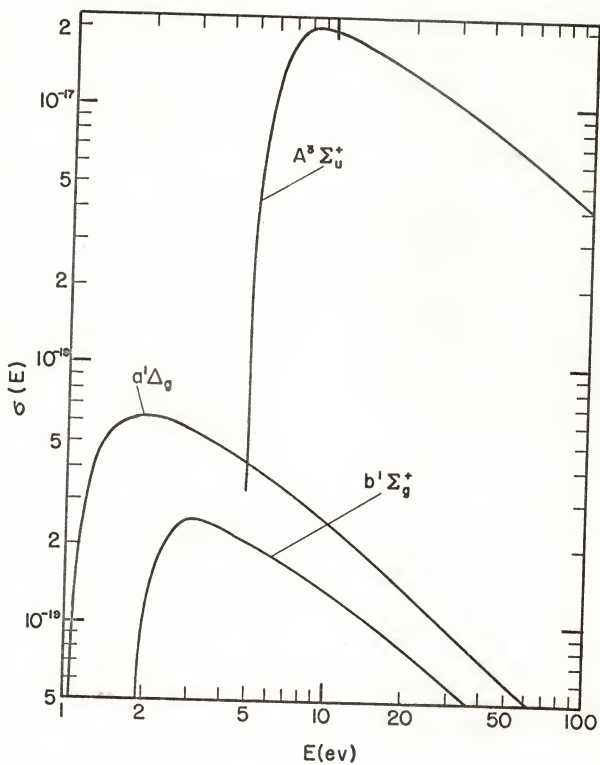


TABLE 12. O_2 Ionization Parameters

State	I	B_0	B_1	B_2	B_3	m	τ	δ	a_3
$X^2\Pi_g$	12.1	0.511	73.6	161	1.56	2.0	2.0	3.0	0.17
$a^4\Pi_u$	16.1	1.07	168	324	3.28	2.0	2.0	3.0	0.17
$A^2\Pi_u$	16.9	0.985	139	274	2.94	2.0	2.0	3.0	0.17
$b^4\Sigma_g^-$	18.2	0.750	107	208	2.29	2.0	2.0	3.0	0.17
B	23.0	0.328	46.9	91	1.002	2.0	2.0	3.0	0.17

TABLE 12. (Continued)

State	C_0	ν	ω	p
$X^2\Pi_g$	.107	3	0.25	1.5
$a^4\Pi_u$	.290	3	0.25	1.5
$A^2\Pi_u$	.274	3	0.25	1.5
$b^4\Sigma_g^-$	.233	3	0.25	1.5
B	.132	3	0.25	1.5

All States

$a_1 = 1.5$

$\alpha_0 = 1.75$

$n_1 = 2.25$

$\alpha_1 = 3.0$

$n_2 = 3.6$

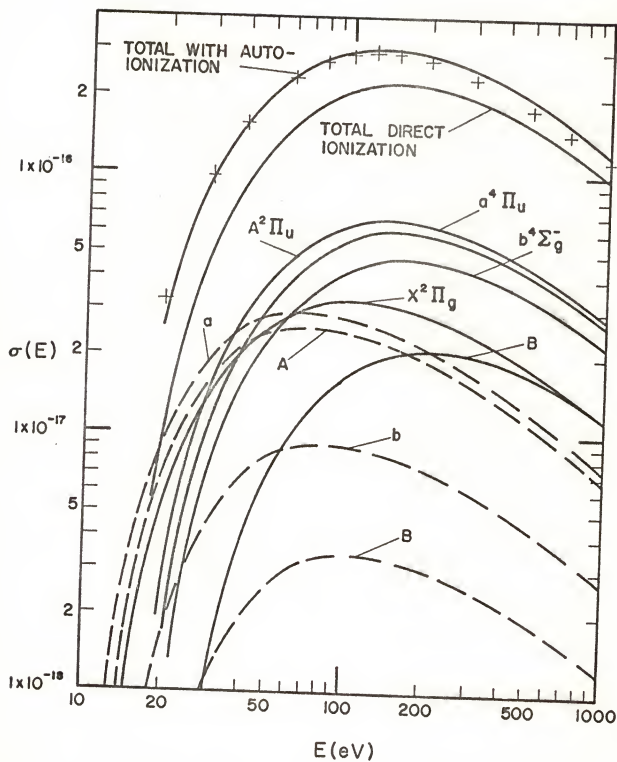
$\alpha_2 = 1.0$

$n_3 = 12.0$

$n_4 = 10.0$

$n_5 = 4.0$

Figure 20. Ionization cross sections. Solid curves are direct ionization, dashed curves are autoionization and crosses are total ionization data of Golden and Rapp.⁵⁴



12.1 eV. The parameters to the simplified forms of Green and Barth¹⁸ are shown in the last three columns of Tables 9, 11 and 12.

5. Vibrational Excitation

Vibrational excitation within the ground state of O_2 occurs in a slightly different way than in N_2 . The compound molecule O_2^- appears at 0.5 eV below the ground state of O_2 . Thus, vibrational excitation proceeding through compound molecule formation is energetically possible at any energy above zero. Data have been given by Schultz⁴⁵ which can be used in conjunction with the absolute total collision cross section of Ramsauer and Kollath⁴⁶ to obtain absolute cross sections for excitation of the ground state vibrations of O_2 . However, we may simulate the average effect of compound molecule formation followed by vibrational excitation of O_2 by assuming there is an effective cross section given by the Green-Barth form with the parameters $W = 0.25$ eV, $C_0 = 9.57 \times 10^{-4}$, $v = 1$, and $\omega = -1$.

CHAPTER V

ENERGY LOSS

1. Energy Loss per cm. Path (Stopping Power)

Consider a gas of a single type of atoms or molecules with number density n . Then an electron of kinetic energy E will lose its energy to excitation states of the atoms or molecules according to

$$-\left(\frac{dE}{dx}\right)_{\text{excitation}} = n \sum_j W_j \sigma_j(E) \quad (1)$$

where j indicates the state of excitation, W_j is the threshold of excitation and $\sigma_j(E)$ is the cross section for excitation of that state. The electron will at the same time lose its energy to ionization according to

$$-\left(\frac{dE}{dx}\right)_{\text{ionization}} = n \sum_i \int_{I_i}^{(E+I_i)/2} W S_i(E, W) dW \quad (2)$$

where i indicates the ionization state, W is the energy loss in a given collision (W = ionization threshold plus secondary electron energy), $S_i(E, W) = \frac{d\sigma_i}{dW}$ is the cross section for losing energy W to the i^{th} state. The upper limit is taken to be $E+I_i/2$ because the electron with the highest energy is taken to be the primary. To obtain the total energy loss per cm. path we simply add the excitation loss to the ionization loss

$$-\frac{dE}{dx} = -\left(\frac{dE}{dx}\right)_{\text{exc}} - \left(\frac{dE}{dx}\right)_{\text{ion}} = n \left[\sum_j W_j \sigma_j(E) + \sum_i \int_{I_i}^{(E+I_i)/2} W S_i(E, W) dW \right]. \quad (3)$$

The assumption has been made here that excitation and ionization are the only processes which contribute significantly to the energy loss in this energy range. The energy range of interest extends from the lowest excitation threshold (about 1 eV) up to the MeV range where radiation by bremsstrahlung becomes important. Since we will consider energies up to only 30 keV we need not consider radiation loss. Below the lowest excitation threshold, loss through elastic collisions and excitation of molecular vibration and rotation becomes important. We will consider these in section 4 of this chapter.

Returning to Eq.(3) and dividing both sides by n we obtain a quantity, called the stopping cross section, which is dependent only on the microscopic properties of the individual atoms or molecules and not on the macroscopic density of the system,

$$L(E) = -\frac{1}{n} \frac{dE}{dx} = \sum_j W_j \sigma_j(E) + \sum_i \int_{I_i}^{(E+I_i)/2} W S_i(E, W) dW \quad (4)$$

which could also be rewritten as

$$L(E) = \sum_j L_j(E) + \sum_i L_i(E) \quad (5)$$

where

$$L_j(E) = W_j \sigma_j(E); \quad L_i(E) = \int_{I_i}^{(E+I_i)/2} W S_i(E, W) dW. \quad (6)$$

We are now in a position to use L_j , L_i and L to determine the amount of energy which an incident electron loses to a particular state while it slows down from its incident energy to below the threshold of the state.

If we consider a gas of more than one constituent we find that the energy loss per centimeter path for each constituent is proportional

to the number density of that constituent. Thus the total energy loss per centimeter path length is for this case

$$-\frac{dE}{dx} = \sum_s n_s \left[\sum_j W_j \sigma_j(E) + \sum_i \int_{I_i}^{E+I_i/2} W S_i(E, W) dW \right]_s \quad (7)$$

where the summation index s refers to the different constituents. Thus $L(E)$ may be written

$$L(E) = -\frac{1}{n} \frac{dE}{dx} = \sum_s \frac{n_s}{n} L_s(E) \quad (8)$$

where $n = \sum_s n_s$ is the total number density. The numbers n_s/n are the fraction 1 number densities of each constituent. For instance, if air is composed of 79% N_2 and 21% O_2 we would have

$$n_{N_2}/n = .79 \quad \text{and} \quad n_{O_2}/n = .21. \quad (9)$$

We now proceed to the discussion of the slowing down process from incident energy to below threshold.

2. Excitation Loss - Electronic States

In this section we will determine the amount of energy which an incident electron loses to the j^{th} electronic state while it slows down from its incident energy to below the threshold energy of the state. For simplicity we will consider a gas of only one constituent. If we divide the stopping cross section for the state by the total stopping cross section, i.e.,

$$f_j(E) = \frac{L_j(E)}{L(E)} = \frac{W_j \sigma_j(E)}{L(E)} \quad (10)$$

we will have the fractional probability $f_j(E)$ of energy going to the j^{th} state while the incident electron is at energy E . Integrating

over the incident particle's energy from its beginning energy E_p down to the threshold for the j^{th} state we have the total energy $E_j(E_p)$ which the incident electron deposits in the j^{th} state during its entire degradation (aside from secondary electrons, of course, which will be considered later). Thus,

$$E_j(E_p) = \int_{W_j}^{E_p} f_j(E) dE = \int_{W_j}^{E_p} \frac{W_j \sigma_j(E) dE}{L(E)}. \quad (11)$$

It should be emphasized that this is the energy deposited by a single electron of energy E_p . If we have a flux of electrons of the single energy E_p we then multiply $E_j(E_p)$ by the flux to obtain the time rate at which energy is being deposited. It is now easy to generalize to an incident flux spectrum. Consider an incident flux $N(E_p) dE_p$ electrons per second in the energy interval E_p to $E_p + dE_p$. Then this incident flux spectrum loses energy to the j^{th} state at the rate

$$E_j(\text{spectrum}) = \int_{W_j}^{\infty} N(E_p) E_j(E_p) dE_p. \quad (12)$$

These considerations of the incident spectrum allow us to consider not only an incident primary spectrum but also the degradation of the secondary electron spectrum. In the next section we will consider the energy loss to ionization and then in Chapter VI we will calculate the energy dependence of the secondary spectrum and its degradation.

The $E_j(E_p)$ functions also allow us to calculate the energy lost by an electron to the j^{th} state as it slows down from any energy E_2 to any other energy E_1 . From Eq.(8) we have

$$\int_{E_1}^{E_2} f_j(E) dE = \int_{W_j}^{E_2} f_j(E) dE - \int_{W_j}^{E_1} f_j(E) dE = E_j(E_2) - E_j(E_1). \quad (13)$$

3. Ionization Loss

The energy loss to ionization can then be obtained in the same way as the excitation of electronic states in Eqs.(7) and (8) of the last section, i.e.,

$$E_i(E_p) = \int_{I_i}^E P f_i(E) dE = \int_{I_i}^E P \frac{\int_{I_i}^{(E+I_i)/2} W S_i(E, W) dW}{L(E)} dE. \quad (14)$$

$E_i(E_p)$ represents the total energy expended in forming ions of the i^{th} state. This energy can then be broken up into two contributions; that which goes into creating the ion, and that which goes to the secondary electron. The energy which goes into the recoil of the ion is small (v_m/M) and can be neglected, as can double ionization and simultaneous excitation - ionization processes. Under these assumptions we rewrite the energy loss W as the sum of the ionization threshold, I_i , and the secondary electron energy, E'

$$W = E' + I_i. \quad (15)$$

Then Eq.(9) becomes

$$E_i(E_p) = \int_{I_i}^E P \frac{\int_{I_i}^{(E+I_i)/2} E' S_i(E, E' + I_i) d(E' + I_i)}{L(E)} dE + \int_{I_i}^E P \frac{I_i \sigma_i(E)}{L(E)} dE \quad (16)$$

where the first term is the energy which goes into secondary electrons while leaving the ion in the i^{th} ionization state and the second term is the energy which goes into the actual creation of the ions during

the entire degradation process. We will subsequently refer to the first term as $E_{\text{sec}_i}(E_p)$ and the second term as $E_{\text{ion}_i}(E_p)$. Thus Eq.(11) may be rewritten as

$$E_i(E_p) = E_{\text{sec}_i}(E_p) + E_{\text{ion}_i}(E_p). \quad (17)$$

At energies more than a few times the lowest ionization threshold it will be found that the largest portion of the energy will be lost to the $E_{\text{sec}_i}(E_p)$ term. This term must then be considered in more detail because the secondaries formed have yet to lose their energy to the gas. The distribution of secondary energies and their degradation will be considered in Chapter VI.

4. Energy Loss of Very Slow Electrons

In this section we mean by "very slow electrons" those whose velocity is below the lowest electronic excitation energy of the gas. These electrons lose energy by three basic processes; 1) vibrational excitation of molecules, 2) rotational excitation of molecules and 3) elastic collisions. The energy loss for such encounters is small and consequently it takes a long time for the electrons to reach thermal equilibrium. At the same time the electrons can travel large distances and collide many times making diffusion an important effect.

We will give only a short discussion of these three types of energy loss here but refer the reader to the article of Crompton and Huxley⁴⁷ in Atomic and Molecular Processes for further discussion and references.

The vibrational excitation of N_2 and O_2 has been considered in Chapters III and IV and parameters for the simplified cross given.

Vibrational excitation of N_2 takes place through the intermediate formation of N_2^- at about 1.4 eV above the zero vibrational level of the ground state. Vibrational excitation of O_2 also takes place through O_2^- but the energy of the ground state of O_2^- is below that of O_2 and hence compound molecule formation takes place very close to zero energy. In the energy loss calculations to follow, only those states lying above the first electronic excitation state at 0198 eV are considered. Thus the O_2 vibrational cross section is not included.

Rotational levels are of the order of hundredths of an eV in spacing and consequently involve very small energy losses. Elastic collisions involve a loss of energy of the order of m/M to the center of mass, where m is the electron mass and M is the mass of the atom or molecule involved.

CHAPTER VI

SECONDARY ELECTRONS

1. Secondary Spectrum

In Chapter IV, section 3, we determined the total energy going into secondary electrons while forming a particular state of the ion. This energy was given by

$$E_{\text{sec}_1}(E_p) = \int_{I_1}^{E_p} \frac{\int_{I_1}^{(E+I_1)/2} E' S_1(E, E'+I_1) d(E'+I_1)}{L(E)} dE. \quad (1)$$

To determine the actual energy spectrum of secondaries we must determine how much energy goes into secondaries in each energy interval E' to $E'+dE'$. To do this we must reverse the order of integration in Eq.(1). Figure 21 shows the region of integration in the E - E' plane. Integrating in the reverse order yields

$$E_{\text{sec}_1}(E_p) = \int_0^{(E_p-I_1)/2} E' dE' \int_{2E'+I_1}^{E_p} \frac{S_1(E, E'+I_1)}{L(E)} dE. \quad (2)$$

We then remove the E' integration and recognize the result as the energy of secondaries in the E' to $E'+dE'$ interval which is just E' times the number of secondaries in the interval. Denoting the number of secondaries in the interval by $n_1(E_p, E')dE'$ we have

$$E' n_1(E_p, E') dE' = E' dE' \int_{2E'+I_1}^{E_p} \frac{S_1(E, E'+I_1)}{L(E)} dE. \quad (3)$$

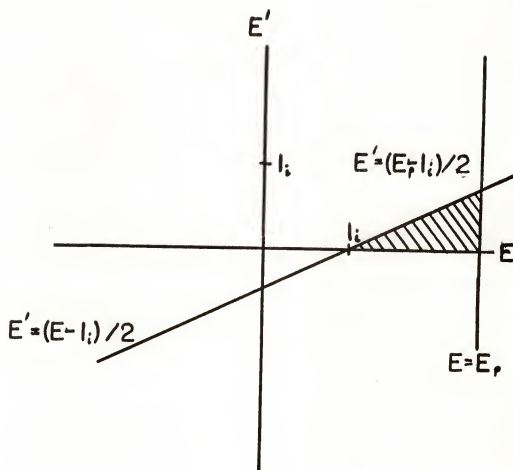


Fig. 21. E - E' integration plane.

Thus the secondary spectrum is given by

$$n_i(E_p, E') = \int_{2E'+I_i}^{E_p} \frac{S_i(E, E'+I_i)}{L(E)} dE. \quad (4)$$

To obtain the total secondary spectrum we sum over all possible ionization states, i

$$n(E_p, E') = \sum_i n_i(E_p, E'). \quad (5)$$

It is seen that a knowledge of the differential (with respect to energy loss) cross section to each ionization state is necessary to know the secondary spectrum. With the knowledge of the spectrum we must now proceed to the consideration of how this spectrum loses its energy.

2. Degradation of Secondary Spectrum

Equation (9) of Chapter V shows how to determine the energy loss to each state for an entire spectrum of energies. Using this equation for the degradation of the secondary spectrum derived in the last section we have

$$E'_j(E_p) = \sum_i \int_{W_j}^{(E_p - I_i)/2} n_i(E_p, E') E'_j(E') dE' \quad (6)$$

where the prime on E_j is used to indicate energy from the secondary spectrum going into the j^{th} state. A simpler equation for calculation can be obtained by noting that the summation and integration can be interchanged if the I_i in the upper limit can be replaced by some average value I . This will be true if $E_p \gg I$. We then have

$$E'_j(E_p) = \int_{W_j}^{(E_p - I)/2} n(E_p, E') E'_j(E') dE'. \quad (7)$$

In the same manner we can determine the energy from the secondary spectrum which goes into the i^{th} ionization state

$$E'_{\text{ion}_i}(E_p) = \int_I^{(E_p - I)/2} n(E_p, E') E_{\text{ion}_i}(E') dE' \quad (8)$$

and into tertiaries from the i^{th} state

$$E'_{\text{sec}_i}(E_p) = \int_I^{(E_p - I)/2} n(E_p, E') E_{\text{sec}_i}(E') dE'. \quad (9)$$

3. Tertiary Spectrum and Its Degradation

Equation (8) tells us the energy in the entire tertiary spectrum of the i^{th} state. To obtain the actual spectrum of energies we must replace $E_{\text{sec}_i}(E')$ by $n_i(E', E'')$ where E'' is the tertiary electron energy and E' is the energy of the secondary electron which ionizes the molecule to form the tertiary. Using a prime as we did above to denote the tertiary spectrum which was formed from the secondary degradation of the tertiary spectrum and denote the resulting quantities by double primes

$$E''_j(E_p) = \int_{W_j}^{(E_p - 3I)/4} n'(E_p, E'') E_j(E'') dE'' \quad (10)$$

$$E''_{\text{ion}_i}(E_p) = \int_{I_i}^{(E_p - 3I)/4} n'(E_p, E'') E_{\text{ion}_i}(E'') dE'' \quad (11)$$

$$E''_{\text{sec}_i}(E_p) = \int_{I_i}^{(E_p - 3I)/4} n'(E_p, E'') E_{\text{sec}_i}(E'') dE''. \quad (12)$$

The upper limit in these three integrals is the maximum energy of the tertiary spectrum which is obtained by taking one half of the difference

of the maximum secondary energy and the average ionization threshold. The maximum secondary energy is $(E_p - I)/2$ and therefore the maximum tertiary energy is

$$\text{Maximum Tertiary Energy} = \frac{\frac{E_p - I}{2} - I}{2} = \frac{E_p - 3I}{4}. \quad (13)$$

4. Summary of Complete Energy Degradation

To obtain the complete energy degradation of an incident electron we must add up the contributions to each state of the successive spectra generated in the manner of the previous sections of this chapter. It is fairly obvious that we could continue the calculation for additional generations of spectra in the same manner but it will be shown in the next chapter that for a 30 keV electron (and hence all lower energies) in N_2 that the process converges sufficiently rapidly to cut off the calculation after the tertiary degradation. Under this assumption, we have for the total energy which goes into the j^{th} excitation state due to the complete energy degradation of an electron with incident energy E_p

$$E_{j \text{ Total}}(E_p) = E_j(E_p) + E'_j(E_p) + E''_j(E_p). \quad (14)$$

Likewise for the i^{th} ionization state we have

$$E_{\text{ion}_i \text{ Total}}(E_p) = E_{\text{ion}_i}(E_p) + E'_{\text{ion}_i}(E_p) + E''_{\text{ion}_i}(E_p). \quad (15)$$

Equations (16) and (17) thus give us the total energy in each state of the atom or molecule and its ion. We can then determine the number of excitations of a particular state by dividing this energy by the excitation threshold for that state. Denoting the number of excitations

by P we have

$$P_j(E_p) = \frac{E_j \text{ Total}(E_p)}{W_j} \quad (16)$$

and

$$P_i(E_p) = \frac{E_{ion_i} \text{ Total}(E_p)}{I_i}. \quad (17)$$

In the next chapter the above considerations will be applied to estimations of auroral and airglow intensities resulting from electron impact excitation.

CHAPTER VII

DEGRADATION IN GASEOUS MIXTURES

1. Energy Transfer Functions

The question of mixtures of gases was touched upon briefly in section 1 of Chapter V and the energy loss was written in terms of the fractional concentrations in Eqs.(7) and (8) of that section. We will now proceed to a more detailed consideration of the actual calculation of the degradation and secondary production in a somewhat realistic gaseous mixture.

The energy transfer functions $E_j(E_p)$ and $E_i(E_p)$ given in Eqs. (12) and (15) of Chapter V were calculated by means of a numerical integration program on an IBM 709 computer. Examples of these curves for some of the states in N_2 , O_2 and O are shown in Figure 22 for a mixture containing 45% N_2 45% O and 10% O_2 . This mixture is representative of an altitude of about 150 km in the atmosphere. These functions while only giving the energy pumped into an excited state from a single particle slowing down, nevertheless contain all the information necessary to calculate the degradation of an entire spectrum and also of any secondary or tertiary spectrum arising. One needs only to fold these functions into the spectrum as was done in Eq.(13) of Chapter V.

Figure 22. Energy transfer curves for selected states
in N_2 , O_2 and O .

2. Secondary Distributions

The basic equations for the calculation of the energy distribution of secondaries were given in Chapter VI. In order to avoid doing a numerical integral for each point on the spectrum, the many-term sum, $L(E)$, was approximated in the following way

$$\frac{1}{L(E)} = \sum_{n=1}^3 c_n \left(\frac{E}{E_u}\right)^{K_n} \quad (1)$$

where $E_u = 1$ eV and the c_n and K_n are adjustable parameters. The function $1/L(E)$ for a 45% N_2 , 45% O and 10% O_2 mixture is shown in Figure 23 along with the approximation of Eq.(1) with $c_1 = 2.3 \times 10^{12}$, $c_2 = 1.09 \times 10^{15}$, $c_3 = 3.3 \times 10^{19}$, $K_1 = 0.715$, $K_2 = -0.528$ and $K_3 = 3.47$. We are now in a position to substitute this approximation into the equations of Chapter VI and carry out the integrals analytically. The secondary spectrum of Chapter VI, Eq.(4) can now be written

$$n_i(E_p, E') = \int_{2E'+I_i}^{E_p} S_i(E, E'+I_i) \sum_{n=1}^3 c_n \left(\frac{E}{E_u}\right)^{K_n} dE \quad (2)$$

where $S_i(E, E'+I_i)$ is given by the simplified form of Eq.(34) of Chapter II. For cases in which S_i has integral v_i as a parameter the integral of Eq.(2) may be carried out analytically to give

$$n_i(E_p, E') = \sum_k b_{ki}(E'+I_i) \eta_{ki} E_p^{\rho_{ki}} \quad (3)$$

where b_{ki} , η_{ki} and ρ_{ki} are combinations of the parameters A_{oi} , I_i , v_i , c_n and K_n . The sum over all ionization states of the secondary spectra for the above mixture is shown in Figure 24 for incident energies $E_p = 30$ keV, 10 keV, 1 keV and 0.1 keV. These spectra can then be folded into the energy transfer functions to obtain the energy

Figure 23. Reciprocal loss function. $1/L(E)$ and its approximation are shown.

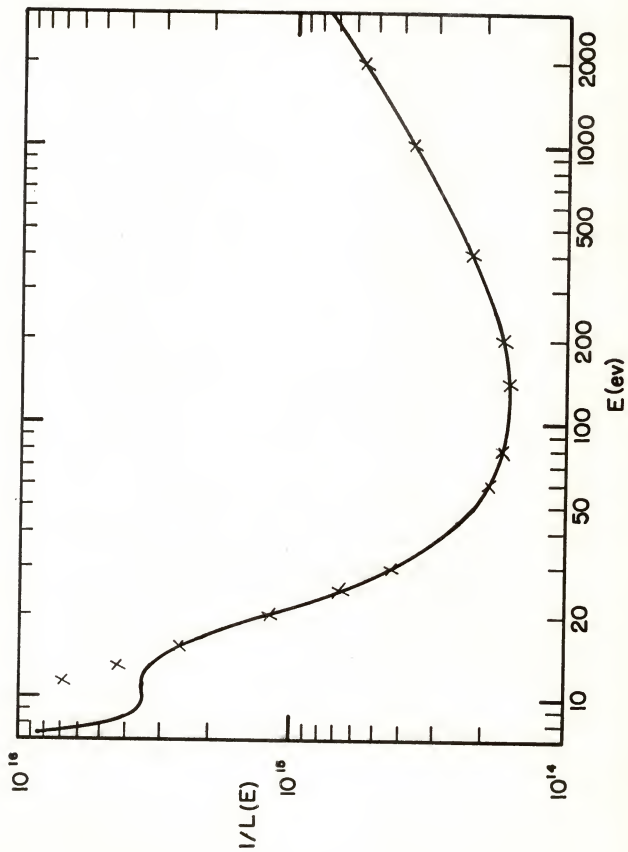
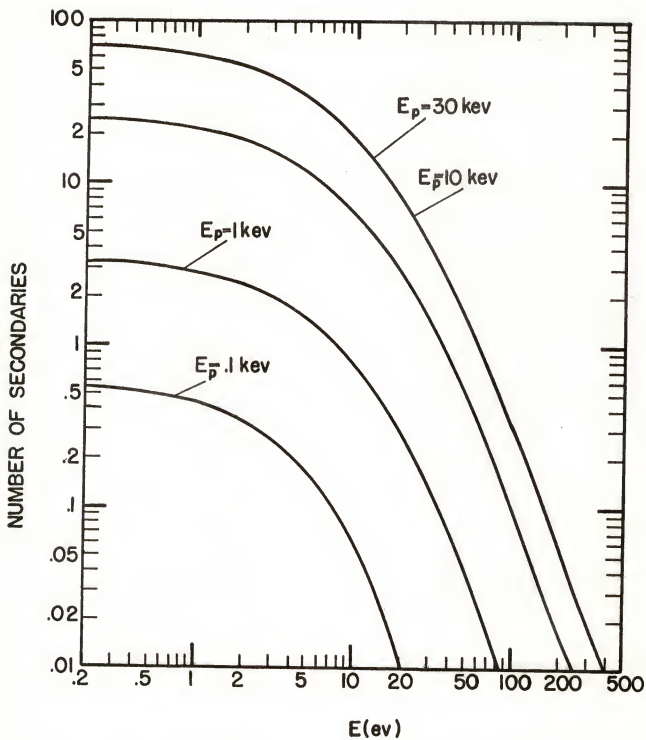


Figure 24. Secondary spectra.



going into each state from the spectra or into themselves to obtain tertiary spectra. The tertiary spectra for each of the four cases of initial energy are shown in Figure 25.

3. Examples of Excited State Population Calculations

a. Photoelectrons

An interesting example of the applicability of the excited state population calculations described above is the degradation of photoelectrons arising from ionization by extreme ultraviolet radiation from the sun. The solar radiation in the extreme ultraviolet region ($< \sim 1000\text{\AA}$) is absorbed in the upper atmosphere mainly by the photoionization process. The photoelectrons thus produced have very low energies in the range of zero to about 400 eV and their degradation gives rise to at least a part of the phenomenon of dayglow. These photoelectrons are produced at altitudes down to about 100 km, with the peak in the production rate occurring at about 150 km.

In order to present a pilot calculation without going into too much detail regarding atmospheric models, we will assume an average relative concentration of the species over the altitude range of 45% N_2 , 45% O and 10% O_2 . The altitude dependence of the excited state population will not be explicitly shown but will instead be integrated. The incident flux of extreme ultraviolet radiation is taken from the tables of Hinteregger, et al.⁴⁸ and the assumption is made that each photon of sufficient energy creates one photoelectron with energy equal to the energy of the photon minus an average ionization potential (15.5 eV). Hinteregger, et al.⁴⁸ give values of the photon flux in

Figure 25. Tertiary spectra.

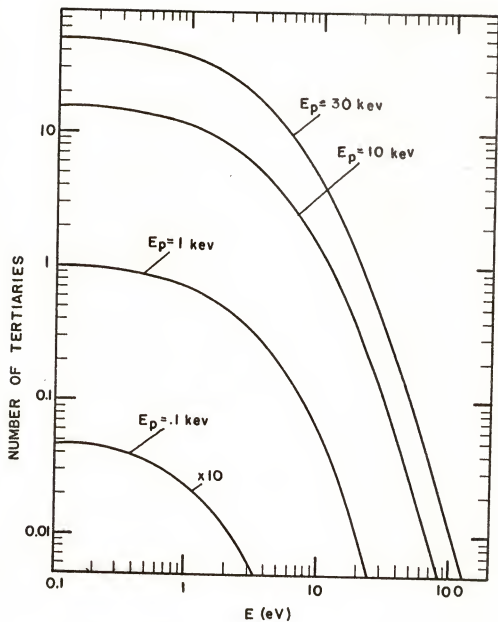


TABLE 13. Photoelectron Groups

Avg. Energy (eV)	No. of Photoelectrons (10^9 electrons)
7.5	9.6
15	3.5
25	7.7
35	2.9
45	2.3
55	5.6
67.5	0.7
90	0.6
120	0.7
160	0.5
235	0.35
235	0.15

various groups and subgroups of energies. Table 13 shows the photoelectron energy groups and photoelectron fluxes under the above assumptions. The degradation of the photoelectron groups was then calculated by means of the energy transfer functions discussed in section 1. When summed over all photoelectron groups this gives the rate at which energy which is pumped into each excited state and dividing by the excitation threshold of the state gives the rate of excitation. These results are shown in Table 14. The effects of secondary electrons will be small.

b. Auroral Electrons

Auroral electrons cover a very wide energy range from a few eV up to many keV. The energy spectrum is not very well known mainly because it can fluctuate greatly from aurora to aurora. In order to present an example of a calculation which could be applied to a realistic spectrum of auroral energies we will consider the degradation of a single electron at four different energies, 30 keV, 10 keV, 1 keV and 0.1 keV. When properly normalized, the degradation results from any one of these energies will give a good first estimate of excitation by a spectrum with that average energy. The results from the degradation at different energies also indicate the energy dependence of the excitations and could be used in the degradation of the spectrum. Alternatively one could use the formulas of Chapters V and VI for the degradation of a spectrum.

Energies in the keV range present a much different and much more difficult problem than the lower energies in the previous section of this chapter. Secondaries and even tertiaries become important in

TABLE 14. Photoelectron Degradation

State *	No. of Excitations	State *	No. of Excitations	State *	No. of Excitations
N ₂	($\times 10^3$)	0		23	0.036
1	16.9	1	0.971	24	0.019
2	14.1	2	0.109	25	0.176
3	3.57	3	0.058	26	0.027
4	3.74	4	0.470	27	0.016
5	1.99	5	0.053	28	0.374
6	1.25	6	0.027	29	0.057
7	3.66	7	0.256	30	0.034
8	0.80	8	0.045	31	0.173
9	0.84	9	0.027	32	0.029
10	1.30	10	0.554	33	0.017
11	0.19	11	0.092	34	0.374
12	0.15	12	0.054	35	0.064
13	0.20	13	0.122	36	0.038
14	0.04	14	0.041	37	0.173
15	0.04	15	0.045	38	0.029
16	1.33	16	0.190	39	0.017
17	0.05	17	0.041	40	0.353
18	0.02	18	0.027	41	0.060
19	0.32	19	0.579	42	0.036
20	0.04	20	0.076	43	0.037
21	0.02	21	0.039	44	0.012
22	80.8	22	0.287	45	0.014

TABLE 14. (Continued)

State *	No. of Excitations	State *	No. of Excitations	State *	No. of Excitations
46	0.018	69	0.006	92	0.019
47	0.006	70	0.163	93	0.022
48	0.007	71	0.024	94	0.027
49	0.056	72	0.014	95	0.010
50	0.019	73	0.069	96	0.010
51	0.021	74	0.013	97	1.031
52	0.028	75	0.007	98	8.701
53	0.009	76	0.143	O ₂	
54	0.010	77	0.026	1	35.7
55	0.029	78	0.015	2	0.15
56	0.010	79	0.069	3	5.28
57	0.011	80	0.013	4	2.63
58	0.014	81	0.007	5	0.24
59	0.005	82	0.146	6	0.20
60	0.005	83	0.026	7	0.11
61	0.244	84	0.016	8	0.68
62	0.031	85	0.019	9	0.10
63	0.017	86	0.007	10	0.09
64	0.116	87	0.008	11	0.58
65	0.015	88	0.009	12	0.09
66	0.008	89	0.003	13	0.09
67	0.078	90	0.004	14	0.13
68	0.012	91	0.056	15	0.03

TABLE 14. (Continued)

State *	No. of Excitations	State *	No. of Excitations
16	0.04	2	0.49
17	0.04	3	0.13
18	0.01	4	0.11
19	0.01	5	0.10
N_2^+		O^+	
1	7.42	1	1.21
2	1.60	2	0.69
3	0.42	3	0.30
4	0.33	O_2^+	
5	0.29	1	0.11
O^+		2	0.15
1	4.14	3	0.13
2	2.24	4	0.09
3	0.93	5	0.03
O_2^+			
1	0.37		
2	0.46		
3	0.38		
4	0.27		
5	0.09		
Secondaries			
N_2^+			
1	2.25		

* State designations are given in Table 15.

this energy range and the methods of Chapter VI are employed to calculate their spectrum of energies.

Tables 15 through 18 show the summarized results of the energy degradation calculation for the four primary energies above. Column 1 of each Table shows the energy deposited in each state directly by the primary electron calculated by Eq.(12) of Chapter V. Column 2 shows the energy deposited in each state by the entire secondary spectrum calculated by Eq.(13) of Chapter VI. Column 3 shows the energy deposited by the entire tertiary spectrum while column 4 shows the sum of columns 1 to 3. Column 5 shows the number of excitations obtained by dividing the total energy by the excitation energy of the state.

Table 19 is a resume of the preceding tables showing the percentage of the total incident energy going into each of the species. It is seen that these percentages remain fairly constant for the 30, 10, and 1 keV cases and then for the 0.1 keV case excitation becomes relatively more important than ionization as would be expected. The small fluctuations can be attributed to the numerical computations which in the degradation of a spectrum may be good to only two or three percent. The column labeled "remainder" is the percentage of the energy which is lost in the interval from zero to about 1 eV through the processes described in Chapter V, section 4. This amount decreases at lower incident energies because of the fewer number of low energy secondaries formed. Table 20 shows the total number of ions formed in each case and the energy per ion pair which is constant at about 32.5 eV/ion pair down to the 1 keV case and has risen to 41.5 eV/ion pair at 0.1 keV.

TABLE 15. Energy Deposition of a 30 keV Electron

State	Primary	Secondary	Tertiary	Total	Number of Excitations
N_2					
1. $A^3\Sigma_u^+$	3.8	1150.	164.	1320.	215.
2. $B^3\Pi_g$	4.2	1100.	135.	1240.	170.
3. $C^3\Pi_u$	1.9	349.	33.2	384.	34.9
4. $a^1\Pi_g$	24.1	302.	26.0	352.	38.7
5. $b^1\Pi_u$	362.	239.	12.3	613.	44.7
6. $h^1\Sigma_u^+$	311.	168.	7.9	487.	34.7
7. $R_X(3)$	695.	446.	22.7	1160.	89.7
8. $R_X(4)$	221.	112.	5.1	338.	23.5
9. $R_X(\text{sum})$	276.	126.	5.5	408.	27.0
10. $R_A(3)$	259.	161.	8.1	428.	32.5
11. $R_A(4)$	63.8	2.9	1.2	94.	6.2
12. $R_A(\text{sum})$	63.5	25.	1.0	99.	6.1
13. $R_B(3)$	75.6	32.	1.3	109.	6.9
14. $R_B(4)$	21.0	7.	0.3	28.	1.6
15. $R_B(\text{sum})$	23.4	7.	0.3	31.	1.7
16. $R_C(3)$	333.	180.	8.4	521.	37.2
17. $R_C(4)$	48.1	12.	0.4	60.	2.9
18. $R_C(\text{sum})$	29.4	6.	0.2	36.	1.6
19. $R_D(3)$	120.	51.	2.1	173.	11.0
20. $R_D(4)$	34.2	9.	0.3	44.	2.2
21. $R_D(\text{sum})$	26.7	6.	0.2	33.	1.5
22. Vibrational	3.3	1540	326.	1870.	1340.

TABLE 15. (Continued)

State	Primary	Secondary	Tertiary	Total	Number of Excitations
0					
1. $3s^3S$	58.5	82.3	6.0	147.	15.4
2. $4s^3S$	14.8	11.7	0.7	27.	2.3
3. ns^3S	11.1	6.9	0.4	18.	1.4
4. $3s^5S$	0.2	39.5	3.9	44.	4.8
5. $4s^5S$	0.04	5.3	0.5	6.	0.5
6. ns^5S	0.02	2.9	0.2	3.	0.2
7. $3p^3P$	4.7	25.4	2.3	39.	3.5
8. $4p^3P$	1.2	4.9	0.4	7.	0.6
9. np^3P	0.9	3.1	0.3	4.	0.3
10. $3p^5P$	0.3	53.6	5.3	59.	5.5
11. $4p^5P$	0.1	9.8	0.9	11.	0.9
12. np^5P	0.04	6.0	0.5	7.	0.6
13. $3d^3D$	17.5	13.3	0.8	31.	2.6
14. $4d^3D$	7.2	4.8	0.3	12.	0.9
15. nd^3D	9.2	5.5	0.3	15.	1.1
16. $3d^5D$	0.1	19.6	1.7	21.	1.7
17. $4d^5D$	0.4	4.4	0.2	5.	0.4
18. nd^5D	0.03	3.0	0.2	3.	0.2
19. $3s^3D$	96.6	66.4	3.8	167.	13.3
20. $4s^3D$	23.9	10.9	0.5	35.	2.3
21. ns^3D	17.5	6.5	0.3	24.	1.5
22. $3s^1D$	0.2	30.6	2.5	33.	2.6

TABLE 15. (Continued)

State	Primary	Secondary	Tertiary	Total	Number of Excitations
23. 4s ¹ D	0.05	4.4	0.3	5.	0.3
24. ns ¹ D	0.03	2.5	0.2	3.	0.4
25. 3p ³ P	7.0	20.8	1.6	29.	2.1
26. 4p ³ P	1.8	3.6	0.3	6.	0.3
27. np ³ P	1.3	2.2	0.2	4.	0.2
28. 3p ¹ P	0.3	43.0	3.6	47.	3.4
29. 4p ¹ P	0.1	7.1	0.5	8.	0.5
30. np ¹ P	0.03	4.4	0.3	5.	0.3
31. 3p ³ D	7.4	20.8	1.6	30.	2.1
32. 4p ³ D	1.9	3.7	0.3	6.	0.4
33. np ³ D	1.4	2.4	0.2	4.	0.2
34. 3p ¹ D	0.3	44.0	3.7	48.	3.4
35. 4p ¹ D	0.1	8.0	0.6	9.	0.6
36. np ¹ D	0.03	4.9	0.4	5.	0.3
37. 3p ³ F	7.4	20.8	1.6	30.	2.1
38. 4p ³ F	1.9	3.8	0.3	6.	0.4
39. np ³ F	1.4	2.4	0.2	4.	0.2
40. 3p ¹ F	0.3	41.4	3.4	45.	3.2
41. 4p ¹ F	0.1	7.5	0.6	8.	0.5
42. np ¹ F	0.03	4.7	0.3	5.	0.3
43. 3d ³ P	12.5	5.4	0.2	18.	1.2
44. 4d ³ P	5.1	2.0	0.1	7.	0.4
45. nd ³ P	6.4	2.3	0.1	9.	0.6

TABLE 15. (Continued)

State	Primary	Secondary	Tertiary	Total	Number of Excitations
46. 3d ¹ P	0.03	2.2	0.2	2.	0.1
47. 4d ¹ P	0.01	0.8	0.1	1.	0.1
48. nd ¹ P	0.01	0.9	0.1	1.	0.1
49. 3d ³ D	19.1	8.3	0.4	28.	1.8
50. 4d ³ D	7.8	3.0	0.1	11.	0.7
51. nd ³ D	9.7	3.5	0.1	13.	0.8
52. 3d ¹ D	0.04	3.4	0.2	4.	0.3
53. 4d ¹ D	0.01	1.2	0.1	1.	0.1
54. nd ¹ D	0.02	1.4	0.1	2.	0.1
55. 3d ³ S	9.9	4.3	0.2	14.	0.9
56. 4d ³ S	4.0	1.6	0.1	6.	0.4
57. nd ³ S	5.0	1.8	0.1	7.	0.4
58. 3d ¹ S	0.02	1.7	0.1	2.	0.1
59. 4d ¹ S	0.01	0.6	0.05	1.	0.1
60. nd ¹ S	0.01	0.7	0.05	1.	0.1
61. 3s ³ P	61.6	32.2	1.6	95.	6.7
62. 4s ³ P	14.9	5.3	0.2	20.	1.2
63. ns ³ P	10.8	3.3	0.1	14.	0.7
64. 3s ¹ P	0.1	13.6	1.0	15.	1.0
65. 4s ¹ P	0.03	2.1	0.1	2.	0.1
66. ns ¹ P	0.04	1.2	0.07	1.	0.1
67. 3p ³ S	4.3	10.0	0.7	15.	1.0
68. 4p ³ S	1.1	1.7	0.1	3.	0.2

TABLE 15. (Continued)

State	Primary	Secondary	Tertiary	Total	Number of Excitations
69. np ³ S	0.7	1.0	0.1	2.	0.1
70. 3p ¹ S	0.1	19.9	1.6	22.	1.5
71. 4p ¹ S	0.03	3.2	0.2	3.	0.2
72. np ¹ S	0.03	2.0	0.1	2.	0.1
73. 3p ³ P	4.6	9.2	0.7	15.	1.0
74. 4p ³ P	1.2	1.8	0.1	3.	0.2
75. np ³ P	0.8	1.1	0.1	2.	0.1
76. 3p ¹ P	0.1	18.1	1.4	20.	1.3
77. 4p ¹ P	0.03	3.5	0.2	4.	0.2
78. np ¹ P	0.03	2.2	0.1	2.	0.1
79. 3p ³ D	4.6	9.2	0.7	15.	1.0
80. 4p ³ D	1.2	1.8	0.1	3.	0.2
81. np ³ D	0.8	1.1	0.07	2.	0.1
82. 3p ¹ D	0.2	18.5	1.4	20.	1.3
83. 4p ¹ D	0.03	3.6	0.2	4.	0.2
84. np ¹ D	0.03	2.2	0.1	2.	0.1
85. 3d ³ P	9.5	3.3	0.1	13.	0.8
86. 4d ³ P	3.9	1.3	0.05	5.	0.3
87. nd ³ P	4.9	1.5	0.05	6.	0.3
88. 3d ¹ P	0.03	1.3	0.07	1.	0.1
89. 4d ¹ P	0.01	0.5	0.03	1.	0.1
90. nd ¹ P	0.02	0.5	0.03	1.	0.1
91. 3d ³ D	27.6	9.6	0.4	38.	2.2

TABLE 15. (Continued)

State	Primary	Secondary	Tertiary	Total	Number of Excitations
92. $4d\ ^3D$	11.3	3.6	0.2	15.	0.8
93. $nd\ ^3D$	14.1	4.3	0.1	18.	1.0
94. $3d\ ^1D$	0.07	3.6	0.2	4.	0.2
95. $4d\ ^1D$	0.02	1.3	0.07	1.	0.1
96. $nd\ ^1D$	0.05	1.5	0.1	2.	0.1
97. $2p\ ^1S$	2.1	48.8	8.1	59.	14.1
98. $2p\ ^1D$	0.6	195.	34.5	230.	121.1
O_2					
1. $a^1\Delta_g$	1.	579.	151.	731.	748.
2. $b^1\Sigma_g^+$	0.01	2.9	0.5	3.	1.9
3. $A^3\Sigma_u^+$	1.9	261.	40.3	303.	67.3
4. $B^3\Sigma_u^-$	74.5	196	15.2	286.	34.0
5. $9.9eV$	9.3	21.2	1.5	32.	3.2
6. $R_X(4)$	17.5	19.2	1.2	38.	3.6
7. $R_X(\text{sum})$	14.0	11.9	0.7	27.	2.3
8. $R_a(3)$	118.	79.8	4.2	202.	15.9
9. $R_a(4)$	30.1	14.8	0.7	46.	3.2
10. $R_a(\text{sum})$	31.4	13.4	0.6	45.	2.9
11. $R_A(3)$	116.	72.0	3.6	192.	14.5
12. $R_A(4)$	31.8	14.1	0.6	47.	3.1
13. $R_A(\text{sum})$	38.9	15.3	0.6	55.	3.4
14. $R_b(3)$	49.6	20.8	0.9	71.	4.5
15. $R_b(4)$	16.5	6.0	0.2	23.	1.4

TABLE 15. (Continued)

State	Primary	Secondary	Tertiary	Total	Number of Excitations
16. $R_b(\text{sum})$	20.9	6.9	0.3	28.	1.6
17. $R_B(3)$	31.2	8.5	0.3	40.	2.0
18. $R_B(4)$	9.1	2.1	0.1	11.	0.5
19. $R_B(\text{sum})$	8.5	1.8	0.1	10.	0.4
N_2^+					
1. $X^2\Sigma_g^+$	3729.	1223.	477.	5000.	321.
2. $A^2\Pi_u$	1031.	294.	107.	1336.	79.8
3. $B^2\Sigma_u^+$	399.	92.	3.	494.	26.3
4. $D^2\Pi_g$	528.	93.	3.	624.	28.4
5. $C^2\Sigma_u^+$	594.	93.	3.	690.	29.2
O^+					
1. ^4S	1277.	557.	25.	1859.	137.
2. ^2D	1496.	418.	15.	1929	114.
3. ^2P	853.	202.	7.	1062.	57.4
O_2^+					
1. $X^2\Pi_g$	134.	46.	2.	182.	15.0
2. $a^4\Pi_u$	448.	88.	3.	539.	33.5
3. $A^2\Pi_u$	438.	79.	2.	519.	30.7
4. $b^4\Sigma_g^-$	393.	63.	2.	458.	25.2
5. B	264.	29.	1.	294.	12.7
Secondaries					
N_2					
1. $X^2\Sigma_g^+$	4607.	464.	13.	5084.	

TABLE 15. (Continued)

State	Primary	Secondary	Tertiary	Total	Number of Excitations
2. $A^2\Pi_u$	1270.	114.	3.	1387.	
3. $B^2\Sigma_u^+$	490.	36.	1.	527.	
4. $D^2\Pi_g$	642.	37.	1.	680.	
5. $C^2\Sigma_u^+$	721.	38.	1.	760.	
0					
1. ^4S	1585.	202.	6.	1793.	
2. ^2D	1842.	162.	4.	2008.	
3. ^2P	1047.	80.	2.	1129.	
O_2					
1. $X^2\Pi_g$	165.	17.	1.	183.	
2. $a^4\Pi_u$	545.	36.	1.	582.	
3. $A^2\Pi_u$	532.	32.	1.	565.	
4. $b^4\Sigma_g^-$	476.	26.	1.	503.	
5. B	315.	12.	0.	327.	

TABLE 16. Energy Deposition of a 10 keV Electron

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
N ₂					
1	3.8	392.	48.8	445.	72.5
2	4.2	372.	39.8	416.	57.0
3	1.9	117.	9.8	129.	11.7
4	12.1	101.	7.6	120.	13.2
5	127.	78.6	3.7	209.	16.3
6	109.	55.3	2.4	166.	11.9
7	244.	147.	6.8	397.	30.5
8	77.2	36.9	1.5	116.	8.1
9	96.2	41.5	1.7	139.	9.2
10	90.7	53.1	2.4	146.	11.1
11	22.2	9.4	0.4	32.	2.1
12	22.1	8.2	0.3	31.	1.9
13	26.3	10.4	0.4	37.	2.3
14	7.3	2.4	0.1	10.	0.6
15	8.1	2.4	0.1	11.	0.6
16	116.	59.1	2.5	178.	12.7
17	16.6	3.9	0.1	21.	1.0
18	10.1	2.1	0.1	12.	0.5
19	41.9	16.6	0.6	59.	3.8
20	11.8	3.0	0.1	15.	0.8
21	9.2	2.1	0.1	17.	0.5
22	3.3	531.	98.4	633.	452.

TABLE 16. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
0					
1	19.7	27.4	1.8	48.9	5.1
2	4.9	3.9	0.2	9.0	0.8
3	3.7	2.3	0.1	6.1	0.5
4	0.2	13.2	1.2	14.6	1.5
5	0.04	1.8	0.1	1.9	0.2
6	0.02	1.0	0.1	1.1	0.1
7	1.7	8.5	0.7	10.9	1.0
8	0.4	1.6	0.1	2.1	0.2
9	0.3	1.0	0.1	1.4	0.1
10	0.3	18.0	1.6	19.9	1.9
11	0.1	3.3	0.3	3.7	0.3
12	0.04	2.0	0.2	2.2	0.2
13	5.8	4.4	0.2	10.4	0.9
14	2.4	1.6	0.1	4.1	0.3
15	3.0	1.8	0.1	4.9	0.4
16	0.1	6.5	0.5	7.1	0.6
17	0.04	1.5	0.1	1.6	0.1
18	0.03	1.0	0.1	1.1	0.1
19	32.1	21.9	1.1	55.1	4.4
20	7.9	3.6	0.2	11.7	0.8
21	5.8	2.1	0.1	8.0	0.5

TABLE 16. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
22	0.2	10.2	0.7	11.1	0.9
23	0.05	1.5	0.1	1.6	0.1
24	0.03	0.8	0.05	0.9	0.1
25	2.4	6.9	0.5	9.8	0.7
26	0.6	1.2	0.1	1.9	0.1
27	0.4	0.7	0.1	1.2	0.1
28	0.3	14.3	1.1	15.7	1.1
29	0.1	2.4	0.1	2.6	0.2
30	0.03	1.5	0.1	1.6	0.1
31	2.5	6.9	0.5	9.9	0.7
32	0.7	1.2	0.1	2.0	0.1
33	0.5	0.8	0.03	1.3	0.1
34	0.3	14.7	1.1	16.1	1.3
35	0.07	2.6	0.2	2.9	0.2
36	0.04	1.7	0.1	1.8	0.2
37	2.6	6.9	0.4	9.9	0.7
38	0.7	1.3	0.07	2.1	0.1
39	0.5	0.8	0.03	1.3	0.1
40	0.3	13.8	1.0	15.1	1.1
41	0.06	2.5	0.2	2.8	0.2
42	0.03	1.6	0.1	1.7	0.1
43	4.1	1.8	0.1	6.0	0.4

TABLE 16. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
44	1.7	0.7	0.03	2.4	0.2
45	2.1	0.8	0.03	2.9	0.2
46	0.03	0.8	0.06	0.9	0.1
47	0.01	0.3	0.02	0.3	0.0
48	0.01	0.3	0.02	0.3	0.0
49	6.3	2.7	0.2	9.2	0.6
50	2.6	1.0	0.05	3.6	0.2
51	3.2	1.2	0.05	4.4	0.3
52	0.05	1.2	0.1	1.3	0.1
53	0.01	0.4	0.02	0.4	0.0
54	0.02	0.5	0.02	0.5	0.0
55	3.3	1.4	0.07	4.8	0.3
56	1.3	0.5	0.02	1.8	0.1
57	1.7	0.6	0.02	2.3	0.1
58	0.02	0.6	0.05	0.7	0.0
59	0.01	0.2	0.01	0.2	0.0
60	0.01	0.2	0.02	0.2	0.0
61	20.4	10.6	0.5	31.5	2.2
62	4.9	1.7	0.1	6.7	0.4
63	3.5	1.1	0.04	4.6	0.3
64	0.1	4.5	0.3	4.9	0.3
65	0.03	0.7	0.04	0.8	0.0

TABLE 16. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
66	0.02	0.4	0.03	0.5	0.0
67	1.5	3.3	0.2	0.5	0.0
68	0.4	0.6	0.04	1.0	0.0
69	0.2	0.4	0.03	0.6	0.0
70	0.1	6.6	0.5	7.2	0.5
71	0.03	1.1	0.06	1.2	0.1
72	0.03	0.6	0.03	0.7	0.0
73	1.6	3.1	0.2	4.9	0.3
74	0.4	0.6	0.04	1.0	0.1
75	0.3	0.4	0.02	0.7	0.0
76	0.1	6.0	0.4	6.5	0.4
77	0.03	1.2	0.07	1.3	0.1
78	0.03	0.7	0.03	0.8	0.0
79	1.6	3.1	0.2	4.9	0.3
80	0.4	0.6	0.04	1.0	0.1
81	0.3	0.4	0.02	0.7	0.0
82	0.2	6.1	0.4	6.7	0.4
83	0.03	1.2	0.07	1.3	0.1
84	0.03	0.7	0.03	0.8	0.0
85	3.1	1.1	0.1	4.3	0.2
86	1.3	0.4	0.3	1.7	0.1
87	1.6	0.5	0.02	2.1	0.1

TABLE 16. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
88	0.03	0.4	0.03	0.5	0.0
89	0.01	0.2	0.01	0.2	0.0
90	0.02	0.2	0.02	0.2	0.0
91	9.1	3.2	0.1	12.4	0.7
92	3.7	1.2	0.07	5.0	0.3
93	4.6	1.4	0.05	6.1	0.3
94	0.07	1.2	0.07	1.3	0.1
95	0.02	0.5	0.02	0.5	0.0
96	0.05	0.5	0.03	0.6	0.0
97	0.7	16.7	2.4	19.8	4.7
98	0.6	66.7	10.4	77.7	40.8
O ₂					
1	1.0	200.	45.9	247.	252.
2	0.01	1.0	0.2	1.2	0.7
3	1.3	89.0	12.1	102.	22.7
4	28.3	65.3	4.5	98.1	11.7
5	3.5	7.0	0.5	11.0	1.1
6	6.2	6.3	0.4	12.9	1.2
7	4.9	3.9	0.2	9.0	0.8
8	41.3	26.3	1.3	68.9	5.4
9	10.5	4.9	0.2	15.6	1.1
10	10.9	4.4	0.2	15.5	1.0

TABLE 16. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
11	40.8	23.7	1.1	65.6	5.0
12	11.1	4.6	0.2	15.9	1.0
13	13.5	5.0	0.2	18.7	1.2
14	17.3	6.9	0.3	24.5	1.6
15	5.7	2.0	0.1	7.8	0.5
16	7.3	2.3	0.1	9.7	0.5
17	10.8	2.8	0.1	13.7	0.7
18	3.1	0.7	0.02	3.8	0.2
19	2.9	0.6	0.02	3.5	0.2
N_2^+					
1	1287.	402.	14.8	1704.	109.
2	355	96.8	3.3	455.	27.2
3	137	30.4	1.0	168.	9.0
4	180.	30.6	0.9	212.	9.6
5	202.	30.9	0.9	234.	9.9
O^+					
1	443.	184.	7.7	634	46.6
2	515.	138.	4.7	657.	38.9
3	293.	66.4	2.1	362.	19.6
O_2^+					
1	46.2	15.2	0.6	62.0	5.1
2	153.	29.2	0.9	183.	11.4

TABLE 16. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
3	149.	26.2	0.8	176.	10.4
4	133.	20.8	0.6	154.	8.5
5	88.7	9.7	0.3	98.7	4.3
Secondaries					
N_2^+					
1	1483.	155.	4.5	1643.	
2	407.	38.1	1.0	446.	
3	156.	12.3	0.3	169.	
4	202.	12.7	0.3	215.	
5	226.	12.9	0.3	239.	
O^+					
1	514.	67.2	2.1	583.	
2	590.	54.4	1.5	646.	
3	333.	26.9	0.7	361.	
O_2^+					
1	53.0	5.8	0.2	59.0	
2	171.	12.2	0.3	184.	
3	167	11.0	0.3	178.	
4	148.	8.8	0.2	157.	
5	96.6	4.2	0.1	101.	

* State designations are given in Table 15.

TABLE 17. Energy Deposition of a 1 keV Electron

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
N_2					
1	3.75	38.47	1.58	43.80	7.13
2	4.22	35.39	1.14	40.75	5.58
3	1.88	10.49	0.22	12.59	1.14
4	3.97	8.65	0.16	12.78	1.40
5	16.40	5.46	0.05	21.91	1.71
6	13.70	3.68	0.03	17.41	1.24
7	31.39	10.14	0.08	41.61	3.20
8	9.65	2.42	0.02	12.09	0.84
9	11.86	2.65	0.02	14.53	0.96
10	11.64	3.64	0.03	15.31	1.16
11	2.74	0.60	0.003	3.34	0.22
12	2.67	0.51	0.002	3.18	0.20
13	3.21	0.65	0.003	3.86	0.25
14	0.87	0.14	0.001	1.01	0.06
15	0.95	0.14	0.0005	1.09	0.06
16	14.65	3.93	0.03	18.61	1.33
17	1.88	0.21	0.0005	2.09	0.10
18	1.12	0.11	0.0002	1.23	0.05
19	5.11	1.04	0.01	6.16	0.39
20	1.35	0.17	.0004	1.52	0.08
21	1.03	0.11	.0002	1.14	0.05
22	3.27	56.21	4.15	59.48	42.49

TABLE 17. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
0					
1	2.64	2.20	0.03	4.87	0.51
2	0.60	0.29	0.003	0.89	0.07
3	0.44	0.16	0.001	0.60	0.04
4	0.21	1.20	0.03	1.44	0.16
5	0.04	0.15	0.003	0.19	0.02
6	0.02	0.08	0.001	0.10	0.01
7	0.32	0.74	0.01	1.07	0.1
8	0.08	0.14	0.002	0.22	0.02
9	0.05	0.09	0.001	0.14	0.01
10	0.28	1.63	0.04	1.91	0.18
11	0.06	0.29	0.01	0.36	0.03
12	0.04	0.18	0.003	0.22	0.02
13	0.71	0.32	0.003	1.03	0.09
14	0.29	0.11	0.001	0.40	0.03
15	0.36	0.13	0.001	0.49	0.04
16	0.14	0.57	0.01	0.72	0.06
17	0.03	0.13	0.002	0.16	0.01
18	0.02	0.09	0.001	0.11	0.01
19	3.88	1.59	0.02	4.49	0.36
20	0.91	0.24	0.02	1.15	0.08
21	0.64	0.13	0.001	0.77	0.05

TABLE 17. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
22	0.23	0.88	0.01	1.12	0.09
23	0.04	0.12	0.002	0.16	0.01
24	0.03	0.07	0.001	0.10	0.01
25	0.40	0.58	0.01	0.99	0.07
26	0.09	0.10	0.001	0.19	0.01
27	0.06	0.06	0.001	0.12	0.01
28	0.28	1.25	0.02	1.55	0.11
29	0.06	0.2	0.003	0.26	0.02
30	0.04	0.12	0.003	0.16	0.01
31	0.42	0.58	0.01	1.00	0.07
32	0.10	0.10	0.001	0.20	0.01
33	0.07	0.06	0.001	0.13	0.01
34	0.28	1.20	0.02	1.50	0.11
35	0.06	0.23	0.004	0.29	0.02
36	0.04	0.14	0.004	0.18	0.01
37	0.42	0.58	0.01	1.00	0.07
38	0.10	0.10	0.001	0.20	0.01
39	0.07	0.06	0.001	0.13	0.01
40	0.28	1.20	0.02	1.50	0.11
41	0.06	0.21	0.003	0.28	0.02
42	0.04	0.13	0.003	0.67	0.04
43	0.47	0.12	0.001	0.59	0.04

TABLE 17. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
44	0.19	0.04	0.0003	0.23	0.01
45	0.23	0.05	0.0003	0.28	0.02
46	0.02	0.06	0.001	0.08	0.01
47	0.01	0.02	0.0003	0.03	0.002
48	0.01	0.02	0.0003	0.04	0.002
49	0.72	0.18	0.001	0.90	0.06
50	0.29	0.06	0.0005	0.35	0.02
51	0.35	0.07	0.0005	0.43	0.03
52	0.04	0.09	0.001	0.13	0.01
53	0.01	0.03	0.0005	0.05	0.003
54	0.02	0.04	0.0005	0.06	0.004
55	0.37	0.09	0.001	0.46	0.03
56	0.15	0.03	0.0002	0.22	0.01
57	0.18	0.04	0.0002	0.07	0.004
58	0.02	0.05	0.001	0.07	0.005
59	0.01	0.02	0.0002	0.02	0.001
60	0.01	0.02	0.0002	0.03	0.002
61	2.38	0.73	0.01	3.02	0.21
62	0.55	0.11	0.001	0.66	0.04
63	0.38	0.06	0.0004	0.45	0.02
64	0.13	0.38	0.01	0.52	0.04
65	0.03	0.05	0.001	0.08	0.005

TABLE 17. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
66	0.02	0.03	0.0004	0.05	0.003
67	0.23	0.27	0.004	0.50	0.03
68	0.05	0.04	0.001	0.10	0.006
69	0.03	0.02	0.0003	0.06	0.003
70	0.15	0.57	0.01	0.73	0.05
71	0.03	0.09	0.001	0.11	0.01
72	0.02	0.05	0.001	0.07	0.004
73	0.24	0.25	0.005	0.45	0.03
74	0.06	0.05	0.001	0.11	0.01
75	0.04	0.03	0.0003	0.07	0.004
76	0.14	0.51	0.005	0.66	0.04
77	0.03	0.10	0.001	0.13	0.01
78	0.02	0.06	0.001	0.08	0.004
79	0.24	0.25	0.005	0.45	0.03
80	0.06	0.05	0.001	0.11	0.01
81	0.04	0.03	0.0003	0.07	0.004
82	0.15	0.52	0.005	0.67	0.04
83	0.03	0.10	0.001	0.13	0.01
84	0.02	0.06	0.001	0.08	0.004
85	0.35	0.07	0.0003	0.41	0.02
86	0.14	0.03	0.0001	0.17	0.01
87	0.17	0.03	0.0002	0.20	0.01

TABLE 17. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
88	0.02	0.03	0.0002	0.05	0.003
89	0.005	0.01	0.0001	0.02	0.001
90	0.01	0.1	0.0002	0.02	0.001
91	1.00	0.19	0.001	1.20	0.07
92	0.41	0.07	0.0003	0.48	0.03
93	0.50	0.09	0.0005	0.59	0.03
94	0.04	0.10	0.001	0.14	0.01
95	0.01	0.04	0.0004	0.05	0.003
96	0.02	0.04	0.0005	0.06	0.003
97	0.18	1.68	0.09	1.95	0.47
98	0.51	6.84	0.39	7.74	4.07
O ₂					
1	1.01	21.94	2.18	25.13	25.64
2	0.01	0.10	0.01	0.12	0.07
3	0.93	8.84	0.42	10.19	2.26
4	4.93	5.36	0.09	10.38	1.24
5	0.60	0.57	0.01	1.18	0.12
6	0.86	0.48	0.01	1.35	0.13
7	0.66	0.29	0.003	0.95	0.08
8	5.36	1.84	0.02	7.22	0.57
9	1.31	0.32	0.002	1.63	0.11
10	1.34	0.28	0.001	1.62	0.10

TABLE 17. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
11	5.23	1.62	0.01	6.86	0.52
12	1.36	0.29	0.002	1.65	0.11
13	1.64	0.31	0.002	1.95	0.12
14	2.10	0.43	0.002	2.53	0.16
15	0.68	0.12	0.001	0.80	0.05
16	0.86	0.13	0.001	0.99	0.06
17	0.24	0.16	0.0004	1.40	0.07
18	0.35	0.04	0.0001	0.39	0.02
19	0.33	0.03	0.0001	0.36	0.02
N_2^+					
1	147.8	24.3	0.1144	172.2	11.05
2	39.9	5.6	0.0217	45.5	2.72
3	14.9	1.7	0.0045	16.6	0.89
4	18.7	1.5	0.0026	20.2	0.92
5	20.6	1.5	0.0020	22.1	0.44
O^+					
1	52.9	11.9	0.0785	64.9	4.77
2	57.7	7.9	0.0299	65.6	3.88
3	32.0	3.6	0.0105	35.6	1.92
O_2^+					
1	5.2	0.9	0.0058	6.1	0.50
2	15.9	1.6	0.0044	17.5	1.09

TABLE 17. (Continued)

State *	Primary	Secondary	Tertiary	Total	Number of Excitations
3	15.3	1.4	0.0033	16.7	0.99
4	13.4	1.0	0.0020	14.4	0.79
5	8.2	0.4	0.0004	8.6	0.37
Secondaries					
N_2^+					
1	119.5	7.5	0.0165	127.02	
2	32.0	1.8	0.0031	33.80	
3	11.7	0.5	0.0007	12.20	
4	14.3	0.5	0.0004	14.80	
5	15.5	0.5	0.0003	16.00	
O^+					
1	43.5	3.5	0.0116	47.01	
2	46.2	2.5	0.0043	48.7	
3	25.2	1.2	0.0015	26.4	
O_2^+					
1	4.2	0.3	0.0009	4.5	
2	12.2	0.5	0.0007	12.7	
3	11.7	0.5	0.0005	12.2	
4	10.1	0.3	0.0003	10.4	
5	5.9	0.1	0.0001	6.0	

* State designations are given in Table 15.

TABLE 18. Energy Deposition of a 0.1 keV Electron

State	Primary	Secondary	Tertiary	Total	No. of Excitations
N_2					
1	3.75	1.59	10^{-4}	5.34	0.87
2	4.22	1.15	10^{-5}	5.37	0.74
3	1.86	0.20	10^{-4}	2.06	0.19
4	2.04	0.15	10^{-8}	2.19	0.24
5	2.61	0.03	0	2.64	0.21
6	1.93	0.01	0	1.94	0.14
7	4.91	0.05	0	4.96	0.38
8	1.31	0.01	0	1.32	0.09
9	1.50	0.01	0	1.51	0.10
10	1.79	0.02	0	1.81	0.14
11	0.34	0.002	0	0.34	0.02
12	0.31	0.001	0	0.31	0.02
13	0.38	0.002	0	0.38	0.02
14	0.09	0.0002	0	0.09	0.01
15	0.09	0.0002	0	0.09	0.005
16	2.06	0.02	0	2.08	0.15
17	0.15	0.0001	0	0.15	0.01
18	0.08	0.00002	0	0.08	0.004
19	0.61	0.003	0	0.61	0.04
20	0.11	0.0001	0	0.11	0.01
21	0.08	0.00004	0	0.08	0.004
22	3.27	3.78	0	7.05	5.04

TABLE 18. (Continued)

State	Primary	Secondary	Tertiary	Total	No. of Excitations
0					
1	0.67	0.03	10^{-10}	0.70	0.07
2	0.11	0.002	0	0.11	0.01
3	0.07	0.001	10^{-8}	0.07	0.01
4	0.20	0.03	0	0.23	0.03
5	0.03	0.002	0	0.03	0.003
6	0.02	0.001	10^{-10}	0.02	0.002
7	0.15	0.01	10^{-10}	0.16	0.01
8	0.03	0.002	0	0.03	0.002
9	0.02	0.001	0	0.02	0.002
10	0.28	0.03	10^{-10}	0.31	0.03
11	0.06	0.005	0	0.06	0.005
12	0.04	0.003	0	0.04	0.003
13	0.13	0.002	0	0.13	0.01
14	0.05	0.001	0	0.05	0.004
15	0.06	0.001	0	0.06	0.005
16	0.13	0.01	0	0.14	0.01
17	0.03	0.002	0	0.03	0.002
18	0.02	0.001	0	0.02	0.002
19	0.68	0.01	0	0.69	0.05
20	0.12	0.001	0	0.12	0.01
21	0.08	0.0003	0	0.08	0.005

TABLE 18. (Continued)

State	Primary	Secondary	Tertiary	Total	No. of Excitations
22	0.21	0.01	0	0.22	0.02
23	0.04	0.001	0	0.04	0.003
24	0.02	0.0005	0	0.02	0.001
25	0.15	0.01	0	0.16	0.01
26	0.03	0.001	0	0.03	0.002
27	0.03	0.001	0	0.02	0.001
28	0.27	0.02	0	0.29	0.02
29	0.05	0.003	0	0.06	0.004
30	0.03	0.001	0	0.03	0.002
31	0.15	0.005	0	0.16	0.01
32	0.03	0.001	0	0.03	0.002
33	0.02	0.001	0	0.02	0.001
34	0.29	0.02	0	0.30	0.02
35	0.06	0.004	0	0.06	0.004
36	0.04	0.001	0	0.04	0.002
37	0.15	0.05	0	0.16	0.01
38	0.03	0.001	0	0.03	0.002
39	0.02	0.001	0	0.02	0.001
40	0.27	0.01	0	0.29	0.02
41	0.06	0.003	0	0.06	0.004
42	0.04	0.001	0	0.04	0.002
43	0.06	0.0003	0	0.06	0.004

TABLE 18. (Continued)

State	Primary	Secondary	Tertiary	Total	No. of Excitations
44	0.02	0.0001	0	0.02	0.001
45	0.03	0.0001	0	0.03	0.002
46	0.02	0.001	0	0.02	0.001
47	0.01	0.0003	0	0.01	0.001
48	0.01	0.0003	0	0.01	0.001
49	0.10	0.0005	0	0.10	0.01
50	0.04	0.0002	0	0.04	0.002
51	0.04	0.0002	0	0.04	0.002
52	0.03	0.001	0	0.03	0.002
53	0.01	0.0005	0	0.01	0.001
54	0.01	0.0005	0	0.01	0.001
55	0.05	0.0002	0	0.05	0.003
56	0.02	0.0001	0	0.02	0.001
57	0.02	0.0001	0	0.02	0.001
58	0.01	0.0005	0	0.01	0.001
59	0.005	0.0002	0	0.005	0.0003
60	0.01	0.0002	0	0.01	0.001
61	0.36	0.003	0	0.36	0.03
62	0.06	0.0003	0	0.06	0.004
63	0.04	0.0001	0	0.04	0.002
64	0.11	0.004	0	0.11	0.01
65	0.02	0.0004	0	0.02	0.001

TABLE 18. (Continued)

State	Primary	Secondary	Tertiary	Total	No. of Excitations
66	0.01	0.0002	0	0.01	0.001
67	0.08	0.003	0	0.08	0.01
68	0.02	0.0003	0	0.02	0.001
69	0.01	0.0003	0	0.01	0.001
70	0.14	0.01	0	0.15	0.01
71	0.02	0.001	0	0.02	0.001
72	0.02	0.0003	0	0.02	0.001
73	0.08	0.003	0	0.08	0.01
74	0.02	0.0003	0	0.02	0.001
75	0.01	0.0003	0	0.01	0.001
76	0.13	0.005	0	0.14	0.01
77	0.03	0.001	0	0.03	0.002
78	0.02	0.0003	0	0.02	0.001
79	0.08	0.003	0	0.08	0.01
80	0.02	0.0003	0	0.02	0.001
81	0.01	0.0003	0	0.01	0.001
82	0.14	0.05	0	0.14	0.01
83	0.03	0.001	0	0.03	0.002
84	0.02	0.0003	0	0.02	0.001
85	0.04	0.0003	0	0.04	0.002
86	0.02	0.0001	0	0.02	0.001
87	0.02	0.00005	0	0.02	0.001

TABLE 18. (Continued)

State	Primary	Secondary	Tertiary	Total	No. of Excitations
88	0.01	0.0003	0	0.01	0.001
89	0.01	0.0001	0	0.01	0.001
90	0.005	0.0001	0	0.05	0.0003
91	0.12	0.001	0	0.12	0.01
92	0.04	0.0001	0	0.04	0.002
93	0.05	0.0001	0	0.05	0.003
94	0.04	0.001	0	0.04	0.002
95	0.01	0.0002	0	0.01	0.001
96	0.01	0.0002	0	0.01	0.001
97	0.14	0.09	10^{-5}	0.23	0.06
98	0.50	0.38	10^{-4}	0.88	0.46
O_2					
1	1.01	1.80	0.014	2.81	2.87
2	0.01	0.01	10^{-6}	0.02	0.01
3	0.83	0.41	10^{-4}	1.24	0.28
4	1.52	0.08	10^{-8}	1.60	0.19
5	0.17	0.01	10^{-11}	0.18	0.02
6	0.18	0.004	10^{-12}	0.18	0.02
7	0.12	0.002	0	0.12	0.01
8	0.87	0.01	0	0.88	0.07
9	0.17	0.001	0	0.17	0.01
10	0.16	0.001	0	0.16	0.01

TABLE 18. (Continued)

State	Primary	Secondary	Tertiary	Total	No. of Excitations
11	0.80	0.01	0	0.81	0.06
12	0.17	0.001	0	0.17	0.01
13	0.19	0.001	0	0.19	0.01
14	0.25	0.001	0	0.25	0.02
15	0.07	0.0002	0	0.07	0.004
16	0.09	0.0002	0	0.09	0.005
17	0.11	0.0001	0	0.11	0.01
18	0.03	0.00001	0	0.03	0.001
19	0.02	0.00001	0	0.02	0.001
N_2^+					
1	14.61	0.0503	0	14.66	0.94
2	3.55	0.0081	0	3.56	0.21
3	1.11	0.0012	0	1.11	0.06
4	1.07	0.0003	0	1.07	0.05
5	1.04	0.0002	0	1.04	0.04
O^+					
1	6.38	0.0439	0	6.42	0.47
2	5.05	0.0109	0	5.06	0.30
3	2.43	0.0029	0	2.43	0.13
O_2^+					
1	0.52	0.0032	0	0.52	0.04
2	1.02	0.0013	0	1.02	0.06

TABLE 18. (Continued)

State	Primary	Secondary	Tertiary	Total	No. of Excitations
3	0.91	0.0009	0	0.91	0.05
4	0.70	0.0004	0	0.70	0.04
5	0.28	0.00002	0	0.28	0.01
Secondaries					
N_2^+					
1	4.67	0.0047	0	4.67	0.30
2	1.10	0.0007	0	1.10	0.07
3	0.33	0.0001	0	0.33	0.02
4	0.29	0.00002	0	0.29	0.01
5	0.27	0.00001	0	0.27	0.01
O^+					
1	2.13	0.0047	0	2.13	0.16
2	1.56	0.0009	0	1.56	0.09
3	0.72	0.0002	0	0.72	0.04
O_2^+					
1	0.18	0.0004	0	0.18	0.01
2	0.31	0.0001	0	0.31	0.02
3	0.27	0.0001	0	0.27	0.02
4	0.20	0.00003	0	0.20	0.01
5	0.07	0.00001	0	0.07	0.003

TABLE 19. Energy into species

Incident Energy	N ₂ (%)	O (%)	O ₂ (%)	N ₂ ⁺ (%)	O ⁺ (%)	O ₂ ⁺ (%)	Remainder
30 keV	32.8	6.1	7.3	27.1	16.2	6.6	3.9
10 keV	33.3	6.1	7.4	27.7	16.5	6.7	2.3
1 keV	34.0	6.1	7.7	27.7	16.6	6.3	1.6
0.1 keV	40.5	11.4	9.1	21.4	13.9	3.4	0.3

TABLE 20. Energy into Ions and eV per Ion Pair

Incident Energy	Number of Ion Pairs	<u>eV</u> Ion Pair	Secondaries	Number of Tertiaries	Quaternaries
30 keV	911	32.9	698	205	8
10 keV	310	32.3	240	67	2
1 keV	31	32.3	27	4	0.01
0.1 keV	2.4	41.5	2.4	0.01	0

TABLE 20. (Continued)

Incident Energy	Secondaries	Average Energy of Tertiaries	Quaternaries
30 keV	20.4	6.2	4.5
10 keV	19.0	6.2	4.5
1 keV	13.1	4.9	2.2
0.1 keV	5.05	1.5	-

This is in very good agreement with experiment. Other energy loss calculations have had much trouble with this point. For instance, Fano⁴⁹ obtained 38 eV/ion pair at 10 keV in helium and Miller³ obtained 46.5 eV/ion pair at 2 keV also in helium. Fano⁴⁹ points out that the large numbers obtained are due to inaccurate accounting for the low energy secondaries formed.

Table 20 also shows the breakdown of the ion formation into the secondary, tertiary and quaternary spectra, showing the rapid convergence of the calculational procedure, and also the average energy of the electrons in their respective spectra.

4. Radiation from Excited States

In order to compare the preceding results with dayglow and auroral measurements it is necessary to determine the rate of radiation from the excited states. This requires the consideration of all of the possible cascading processes and their branching ratios. Eleven of the important lines of atomic oxygen are considered and these are given in Table 21 under the heading "transition". The intensities of these lines are calculated using the equations of Barth⁵⁰ which are

$$4\pi I_{1304} = N_1 + N_2 + N_3 + N_7 + N_8 + N_9 + 0.376 N_{13} + N_{14} + N_{15} + 0.112 [N_{19} + N_{20} + N_{21} + N_{25} + N_{26} + N_{27} + N_{31} + N_{32} + N_{33} + N_{37} + N_{38} + N_{39} + N_{49} + N_{50} + N_{51} + N_{55} + N_{56} + N_{57}] \quad (4)$$

$$4\pi I_{8446} = 4\pi I_{1304} - N_1 - N_8 - N_9 - N_{15} \quad (5)$$

$$4\pi I_{1356} = N_4 + N_5 + N_6 + N_{10} + N_{11} + N_{16} + N_{17} + N_{18} \quad (6)$$

TABLE 21. Airglow Features

Transition Atomic Oxygen	λ ($\text{\AA}$)	Number of Quanta Radiated ($10^9/\text{cm}^2\text{sec}$)
$^3\text{S} \rightarrow ^3\text{P}$	1304	1.77
$^3\text{P} \rightarrow ^3\text{S}$	8446	0.68
$^5\text{S} \rightarrow ^3\text{P}$	1356	1.04
$^5\text{P} \rightarrow ^5\text{S}$	7773	0.89
$^3\text{D} \rightarrow ^3\text{P}$	1027	0.08
$^3\text{D} \rightarrow ^3\text{P}$	989	1.33
$^1\text{D} \rightarrow ^1\text{D}$	1152	1.12
$^1\text{P} \rightarrow ^1\text{S}$	1218	0.24
$^1\text{P} \rightarrow ^1\text{D}$	998	0.47
$^1\text{S} \rightarrow ^1\text{D}$	5577	1.21
$^1\text{D} \rightarrow ^3\text{P}$	6300	11.4
	*	0.20
N_2		
$\text{B}^2\Sigma_u^+ \rightarrow \text{X}^2\Sigma_g^+$	1st Neg.	0.42
$\text{A}^2\Pi_u \rightarrow \text{X}^2\Sigma_g^+$	Meinel	1.89
$\text{A}^3\Sigma_u^+ \rightarrow \text{X}^1\Sigma_g^+$	Vegard-Kaplan	34.5
	*	4.31
$\text{B}^3\Pi_g \rightarrow \text{A}^3\Sigma_u^+$	1st Pos.	17.7
$\text{C}^3\Pi_u \rightarrow \text{B}^3\Pi_g$	2nd Pos.	3.57
$\text{a}^1\Pi_g \rightarrow \text{X}^1\Sigma_g^+$	LBH	{ 10.7 14.1
$\text{b}^1\Pi_u \rightarrow \text{X}^1\Sigma_g^+$	BH	
$\text{b}^1\Pi_u \rightarrow \text{a}^1\Pi_g$	Janin	} 6.95
$\text{h}^1\Sigma_u^+ \rightarrow \text{X}^1\Sigma_g^+$	Watson-Koontz	
$\text{h}^1\Sigma_u^+ \rightarrow \text{a}^1\Pi_g$	Herman-Gaydon	} 3.37
O_2		
$\text{A}^2\Pi_u \rightarrow \text{X}^2\Pi_g$	2nd Neg.	0.38
$\text{b}^4\Sigma_g^- \rightarrow \text{a}^4\Pi_u$	1st Neg.	0.27

TABLE 21. (Continued)

Transition Atomic Oxygen	λ (Å)	Number of Quanta Radiated ($10^9/\text{cm}^2\text{sec}$)
$a^1\Delta_g \rightarrow X^3\Sigma_g^-$	IR Atm.	35.7
	*	20.7
$b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$	Atm.	0.15

* Corrected for quenching.

$$4\pi I_{7773} = N_5 + N_6 + N_{10} + N_{16} + N_{17} + N_{18} \quad (7)$$

$$4\pi I_{1027} = 0.624 N_{13} \quad (8)$$

$$4\pi I_{989} = 0.888 [N_{19} + N_{20} + N_{21} + N_{25} + N_{26} + N_{27} + N_{31} + N_{32} + N_{33} \quad (9)$$

$$+ N_{37} + N_{38} + N_{39} + N_{49} + N_{50} + N_{51} + N_{56} + N_{57}]$$

$$4\pi I_{1152} = N_{22} + N_{23} + N_{24} + N_{28} + N_{29} + N_{30} + N_{34} + N_{35} + N_{36} + N_{40} + N_{41} + N_{42} \quad (10)$$

$$4\pi I_{1218} = 0.339 [N_{64} + N_{65} + N_{66} + N_{70} + N_{71} + N_{72} + N_{76} + N_{77} + N_{78} + N_{82} + N_{83} + N_{84}] \quad (11)$$

$$4\pi I_{998} = 1 - 4\pi I_{1218} \quad (12)$$

$$4\pi I_{5577} = 0.952 [N_{97} + 4\pi I_{1218}] \quad (13)$$

$$4\pi I_{6300} = N_{98} + N_{22} + N_{28} + N_{34} + 4\pi I_{998} + 4\pi I_{5577} \quad (14)$$

where N_n is the number of atoms in the n^{th} excited state and the coefficients are the branching ratios. The subscripts n refer to the states listed in Table 15. Table 21 also shows the N_2 and O_2 transitions considered. The cascading for N_2 was considered in the same way as done by Green and Barth.¹⁸ The two possibilities shown for the Lyman-Birge-Hopfield bands are respectively, the direct contribution of the $a^1\pi_g$ plus the cascading contribution of the $b^1\pi_u$ through the Janin bands and the direct contribution of the $a^1\pi_g$ plus the $b^1\pi_u$

plus the cascading contribution of the $h^1\Sigma_u^+$ through the Gaydon-Herman bands. The transitions in O_2 were obtained from Chamberlain's⁵¹ diagram. Table 21 shows the results of the dayglow calculation with these cascading processes considered.

The first four columns of Table 22 show the number of radiated quanta per incident electron for each of the four auroral cases considered. In order to obtain comparison with experiment first negative bands of N_2 are normalized to Chamberlain's⁵¹ value of 165 kR for an IBC III aurora. The results are shown in the next four columns of Table 22 while the last 2 columns show the experimental results given by Chamberlain⁵¹ and Crosswhite, et al.⁵²

5. Corrections for Quenching

The transitions marked by asterisks in Tables 21 and 22 have been corrected for quenching (or collisional deactivation). For long-lived metastables the possibility of depopulation by collision with neutral gas particles rather than by radiation is always a possibility. To investigate its importance consider the total rate of depopulation of an excited state

$$\frac{dn^*}{dt} = An^* + \sum_x n_x^* k_x^* \quad (15)$$

where A is the Einstein coefficient for radiation, x indicates the quenching species, n_x is the number density of the quenching species and k_x is the quenching coefficient. The fraction of the depopulations which give rise to radiation is

$$F = \frac{An^*}{An^* + \sum_x n_x^* k_x^*} \quad (16)$$

TABLE 22. Auroral Features

Transition	Number of Quanta Radiated per Electron				
	λ	30 keV	10 keV	1 keV	0.1 keV
Atomic Oxygen	1304	29.6	9.93	0.95	0.131
	8446	13.8	4.13	0.38	0.052
	1356	14.7	5.0	0.50	0.087
	7773	0.6	0.19	0.02	0.004
	1027	1.6	0.56	0.06	0.01
	989	26.5	9.41	0.82	0.11
	1152	15.9	5.8	0.53	0.102
	1218	2.1	0.64	0.07	0.017
	998	4.1	1.3	0.15	0.020
	5577	15.4	5.1	0.52	0.073
	{ 6300	150.0	50.4	4.74	0.57
	{ *				
N_2					
1st Negative		26.3	9.0	0.89	0.06
Meinel		109.	37.1	3.66	0.25
Vegard-Kaplan	{	420	141.	13.86	1.80
	{ *				
1st Positive		205.	68.7	6.72	0.93
2nd Positive		34.9	11.7	1.14	0.19
Lyman-Birge-Hopfield	{	209	71.1	7.46	0.97
	{	304	103.8	10.87	1.35
Birge-Hopfield	}				
Janin		170.	57.9	6.06	0.73
Watson-Koontz	}				
Herman-Gaydon		95.4	32.7	3.41	0.38
O_2					
2nd Negative		30.7	10.4	0.99	0.05
1st Negative		25.2	8.5	0.79	0.04
IR Atmospheric	{	748.	252.	25.64	2.87
	{ *				
Atmospheric		2.1	0.74	0.07	0.01

TABLE 22. (Continued)

Transition	Intensity of IBC III Aurora				Experimental Results	
	30 keV	10 keV	1 keV	0.1 keV	Chamberlain	Crosswhite <u>et al.</u>
Atomic Oxygen	184	182	176	360		
	86	76	71	143		
	92	92	93	240		
	4	4	4	11		
	10	10	11	27		
	165	172	152	303		
	99	106	98	280		
	13	12	13	47		
	25	24	26	50		
	96	94	97	200	100	
	{ 930	920	880	1570		
	*17	16	16	28	50	
N_2						
1 Neg.	165	165	165	165	165	
Meinel	680	680	680	690	2500	
VK	{ 2610	2590	2570	4950		
	*330	320	320	630	150 ⁺	30 - 120 ⁺
1st Pos.	1270	1260	1250	2560	2000	
2nd Pos.	217	215	212	523	100	
LBH	{ 1300	1300	1380	2670		
	1890	1900	2020	3720		450 - 1850
BH	} 1060	1060	1120	2010		
Janin						
WK	} 590	600	630	1050		
HG						
O_2						
2nd Neg.	191	191	183	137		
1st Neg.	157	156	146	110	10	
IR Atm.	{ 4650	4610	4940	7900		
	*2700	2680	2870	7600	1000	
Atm.	13	14	13	27	400	

* Corrected for Quenching

[†] Chamberlain's value of the Vegard-Kaplan intensity includes only those bands longward of 3000 Å, the value of Crosswhite, et al. includes only those shortward of 2600 Å.

or upon simplification

$$F = \frac{1}{1 + \frac{\sum_n k}{A}} \quad (17)$$

The quenching coefficients were obtained from Hunten and McElroy.⁵³

The Einstein coefficients are approximately given by the reciprocal of the lifetimes. The densities used to calculate these quenching corrections were 10^{10} particles/cm³ for O and N₂ and 10^9 particles/cm³ for O₂. The quenching coefficients and resulting corrections are shown in Table 23 for five transitions. It can be seen that the largest correction is obtained for the ¹D → ³P transition in O and is 1/56.

6. Discussion of Results

The dayglow results are fairly inconclusive in that they are not in a form readily comparable to experiment. It is necessary to calculate altitude profiles or intensities in order to be able to compare with the rocket and satellite measurements. A paper is now in progress concerning these points with Professor Green and Professor C. A. Barth of the University of Colorado.

The auroral results for the 30, 10 and 1 keV cases are almost identical while the 0.1 keV case gives results which are significantly larger for most lines. This is because the first negative band in N₂⁺ was chosen for normalization and it was noted earlier that at this incident energy ionization is relatively less important than at the higher energies. Note that most of the predicted intensities are within factors of 3 or 4 of the measured values with notable exceptions in O₂. In particular the atmospheric bands arising from the b¹Σ_g⁺ state

TABLE 23. Quenching Coefficients and Corrections

Transition	Lifetime (sec.)	A	k_{N_2}	k_O	k_{O_2}	F
$O^1D \rightarrow ^3P$	110	$\frac{1}{110}$	5×10^{-11}	1.6×10^{-13}	4×10^{-15}	$\frac{1}{56}$
$O^1S \rightarrow ^1D$	0.74	$\frac{1}{0.74}$	10^{-16}	1.6×10^{-13}	4×10^{-15}	1
$O_2 a^1\Delta_g \rightarrow X^3\Sigma_g^-$	3600	$\frac{1}{3600}$	2×10^{-19}	2×10^{-14}	2×10^{-19}	$\frac{1}{1.7}$
$O_2 b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$	7	$\frac{1}{7}$	10^{-16}	10^{-15}	10^{-16}	1
N_2 Vegard-Kaplan	10	$\frac{1}{10}$	3×10^{-19}	3×10^{-11}	4×10^{-10}	$\frac{1}{8}$

gives a very small intensity in our calculation. This could be due either to an incorrect cross section or to some other unaccounted for process which contributes to the intensity of the bands.

The autoionization cross sections determined in Chapters III and IV have not been considered to add to the continuum or the secondary spectra in the degradation calculation. They were found to contain only about 1% of the incident energy and this energy was vested in secondary electrons in the 0 - 10 eV range with most of them falling in the 0 - 2 eV range. Hence, most of their energy falls in the range below our degradation calculations. It is fairly obvious that the next generation of degradation calculations should consider the 0 - 2 eV range in greater detail and consider all of the relevant processes in that range.

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BIOGRAPHICAL SKETCH

Richard Stanley Stolarski was born on November 22, 1941 at Fort Lewis, Washington. He was graduated from Wilson High School of Tacoma, Washington in June, 1959. In June, 1963 he received the degree of Bachelor of Science with honors in physics and mathematics from the University of Puget Sound, also in Tacoma. From September, 1966 until the present time he has pursued his work toward the degree of Doctor of Philosophy in physics at the University of Florida. During this time he held a graduate assistantship, graduate school fellowship and NASA traineeship.

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This dissertation was prepared under the direction of the chairman of the candidate's supervisory committee and has been approved by all members of that committee. It was submitted to the Dean of the College of Arts and Sciences and to the Graduate Council, and was approved as partial fulfillment of the requirements for the degree of Doctor of Philosophy.

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